

## Supporting Information

### Design, synthesis and structure-activity relationships of mangostin analogs as cytotoxic agents

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### Abbreviation for the manuscript

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DCM	Dichloromethane
DMF	Dimethylformamide
BrBn	Benzyl bromide
DMAP	4-Dimethylaminopyridine
Ac <sub>2</sub> O	Acetic anhydride
(CH <sub>3</sub> ) <sub>2</sub> SO <sub>4</sub>	Dimethyl sulfate
BrCH <sub>2</sub> CHCH <sub>2</sub>	3-Bromopropene
BrCH <sub>2</sub> CHC(CH <sub>3</sub> ) <sub>2</sub>	1-Bromo-3-methyl-2-butene
OsO <sub>4</sub>	Osmium tetroxide
NMO	4-Methylmorpholine-N-oxide
DDQ	2,3-Dicyano-5,6-dichlorobenzoquinone

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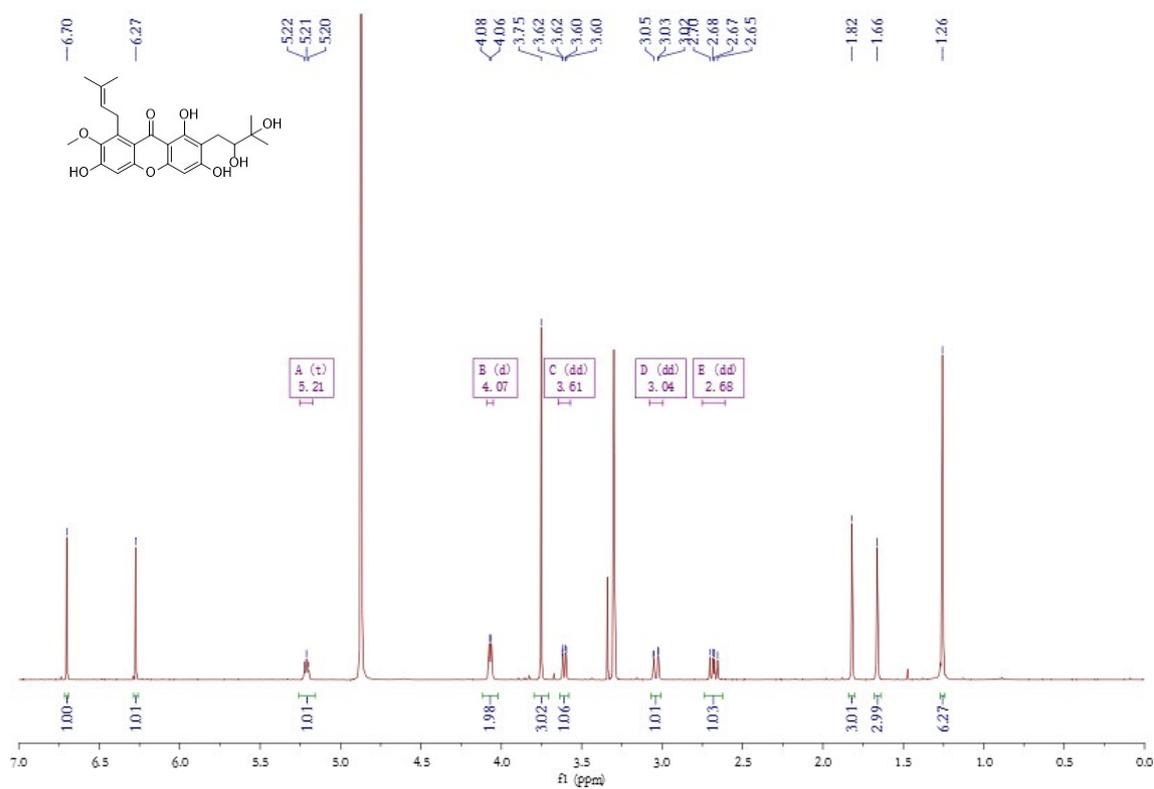


Figure 1S.  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 500 MHz) of compound 2a

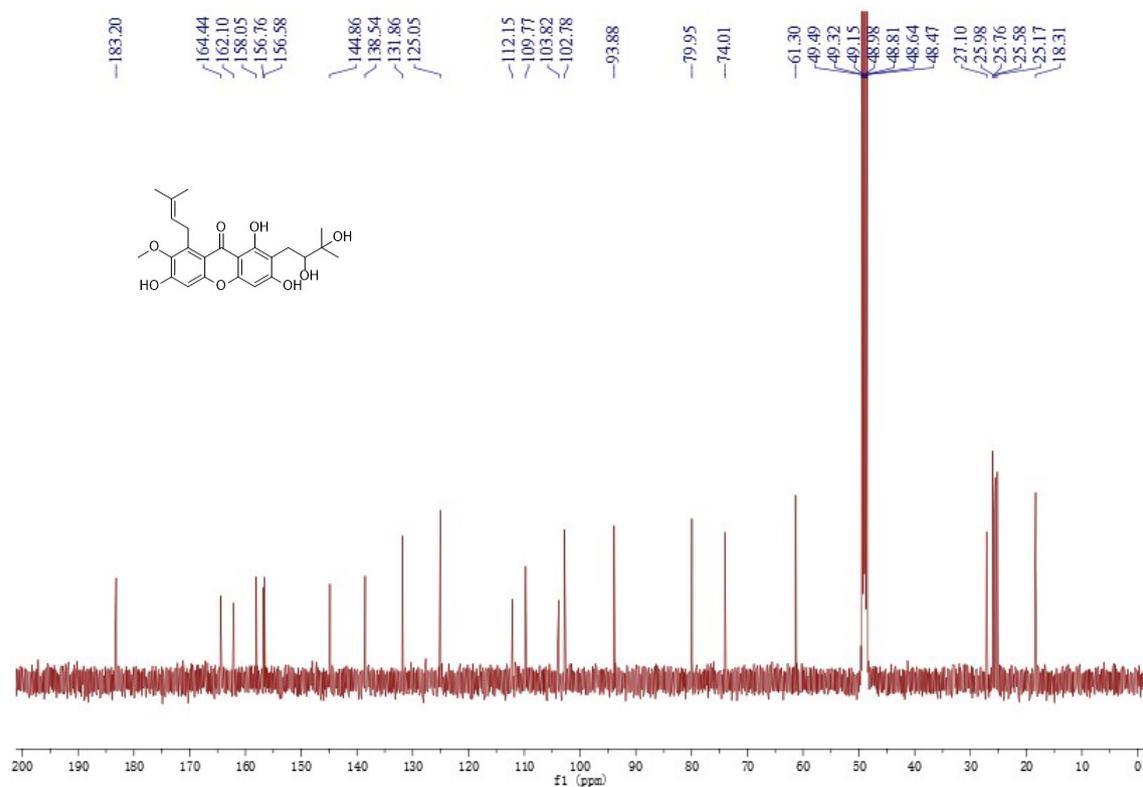
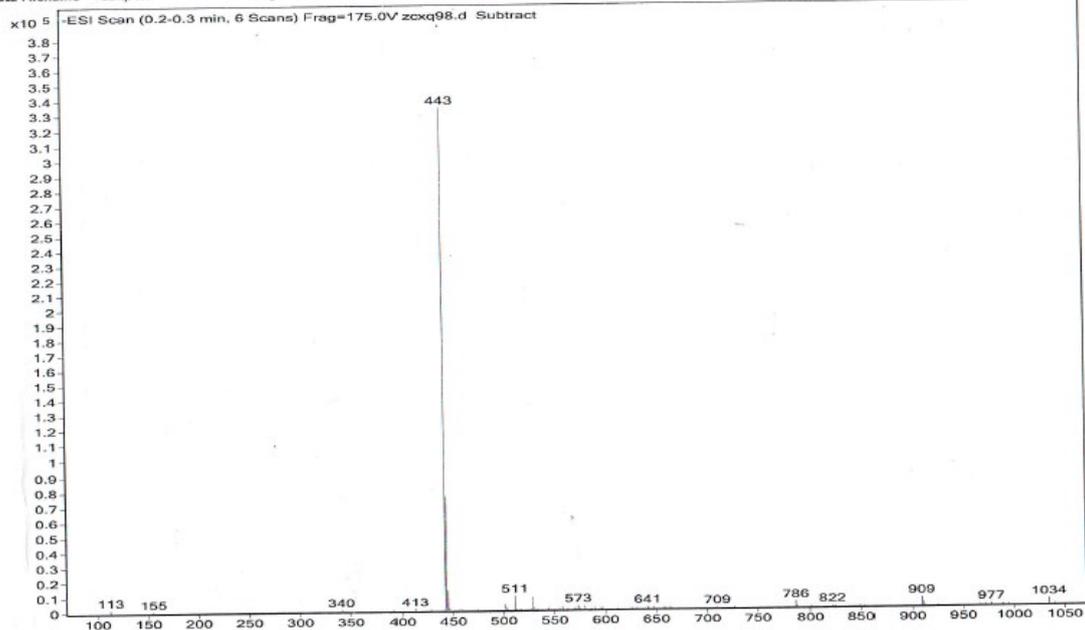
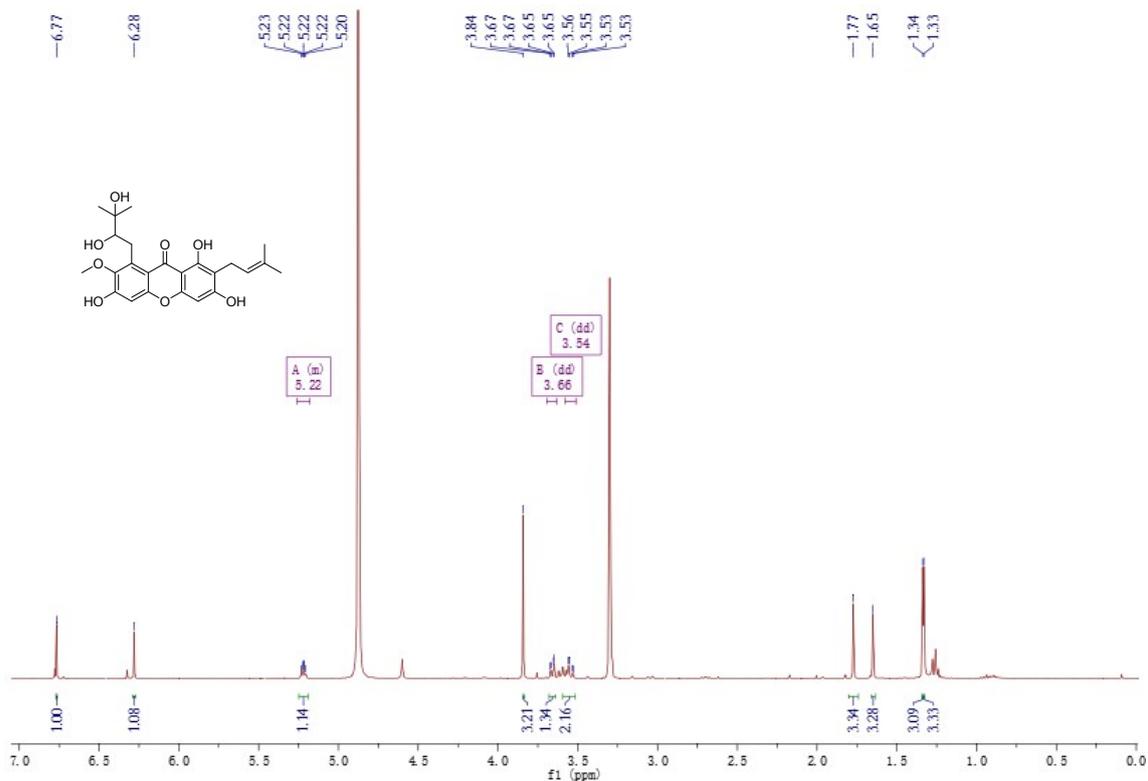


Figure 2S.  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 125 MHz) of compound 2a

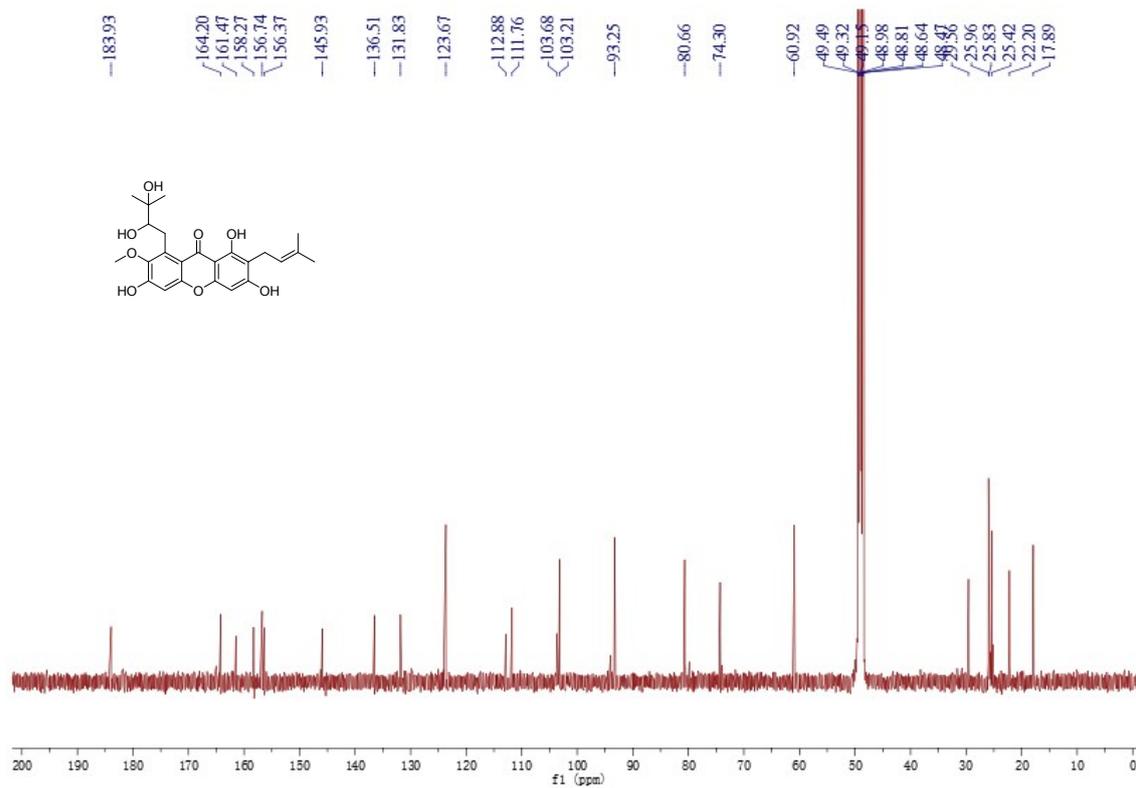
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Inj Vol	0.1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	zcxq98.d	ACQ Method	SIBU-ESI-4m	Comment		Acquired Time	11/2/2016 3:10:11 PM



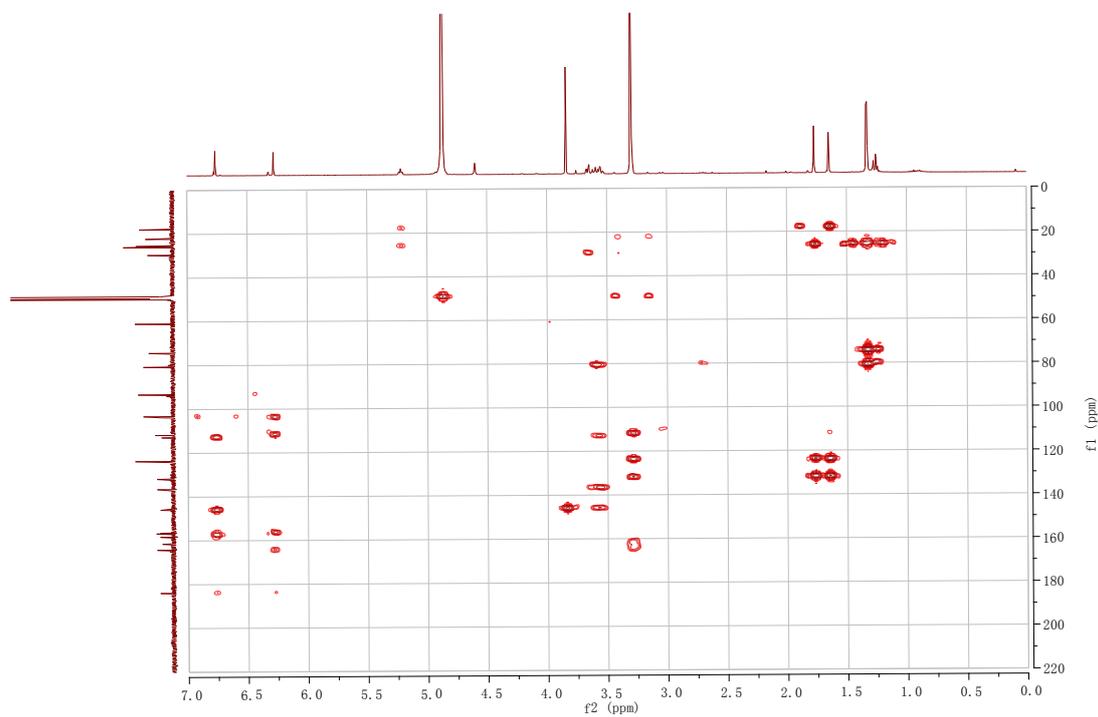
**Figure 3S.** Negative ESI-MS spectrum of compound **2a**



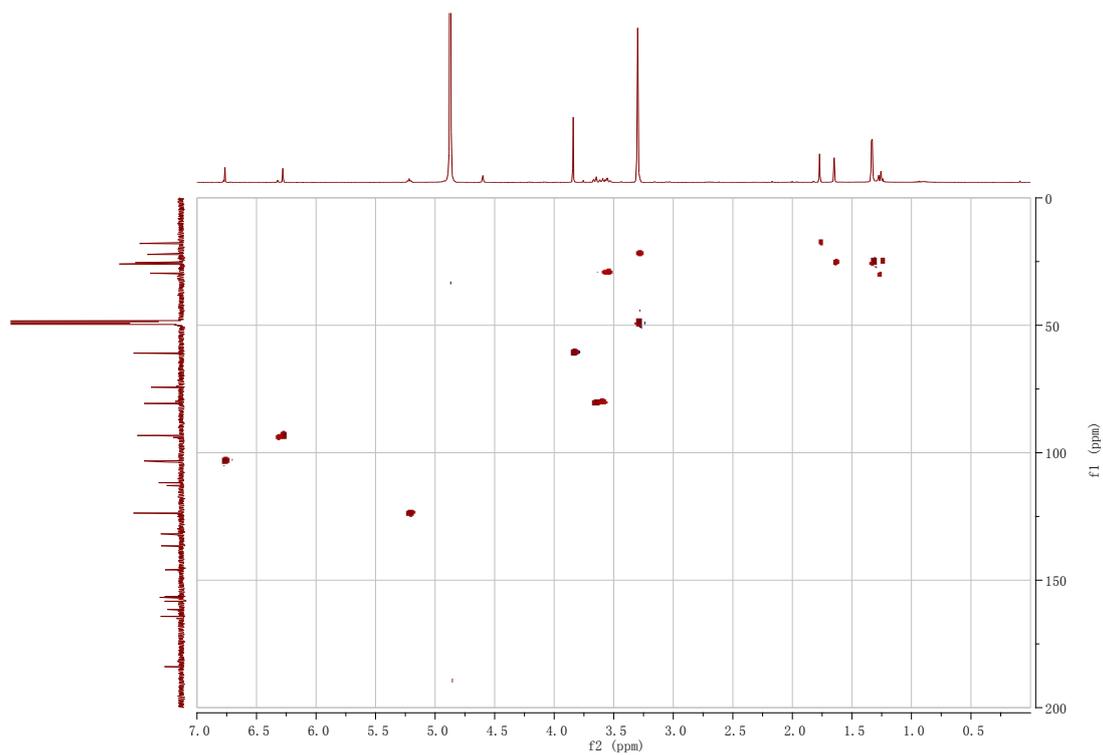
**Figure 4S.**  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 500 MHz) of compound **2b**



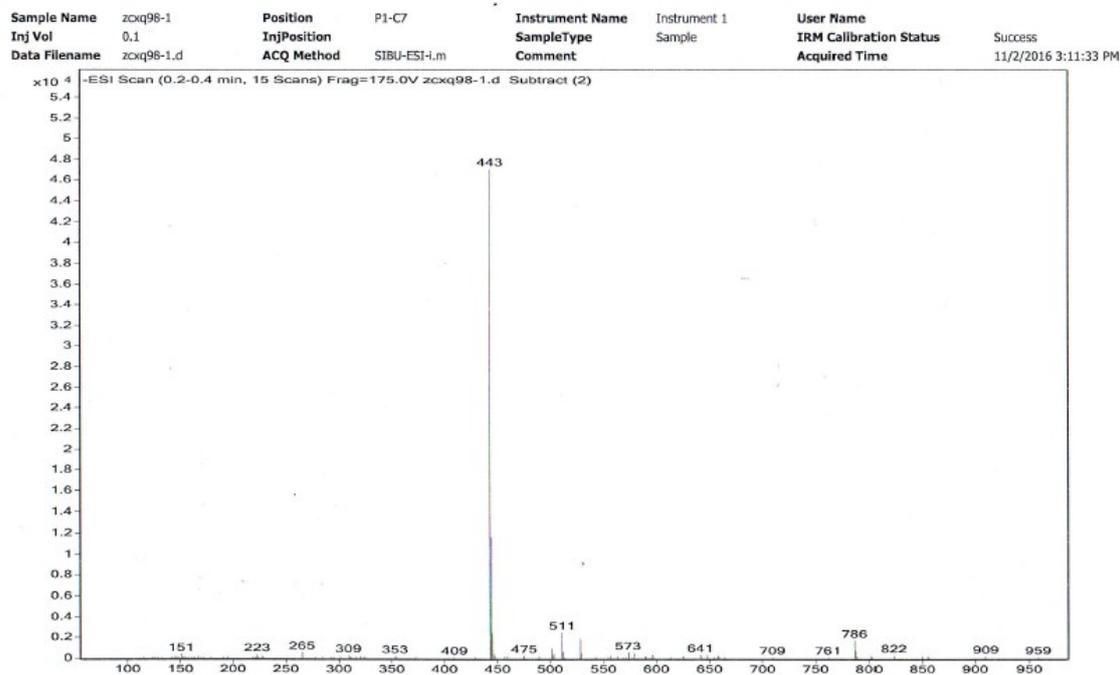
**Figure 5S.**  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 125 MHz) of compound **2b**



**Figure 6S.** HMBC spectrum ( $\text{CD}_3\text{OD}$ , 125 MHz) of compound **2b**



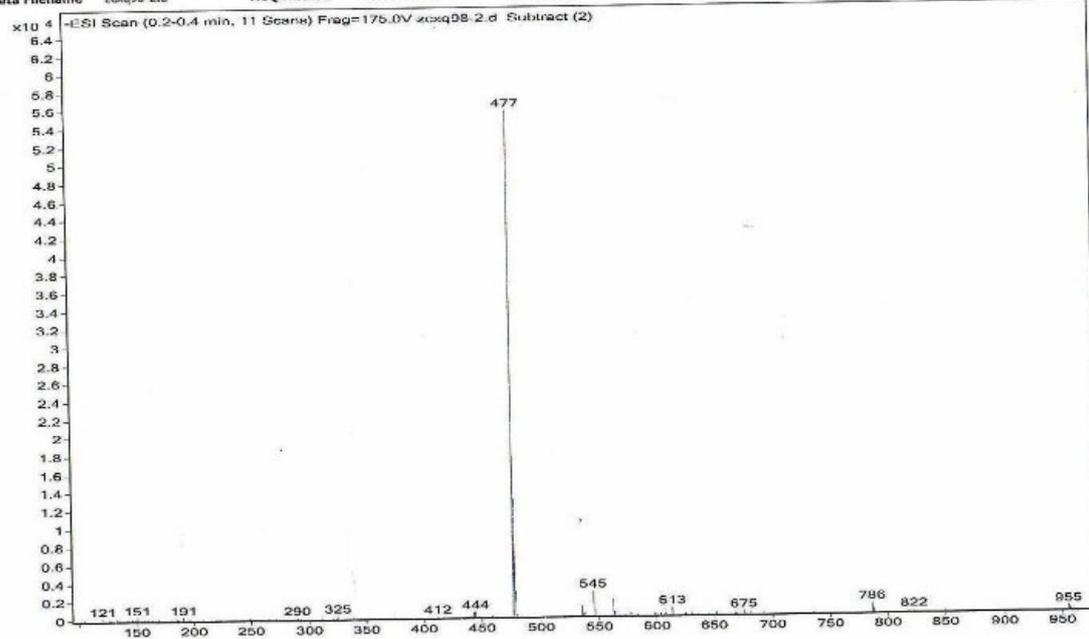
**Figure 7S.** HSQC spectrum (CD<sub>3</sub>OD, 125 MHz) of compound **2b**



**Figure 8S.** Negative ESI-MS spectrum of compound **2b**



Sample Name	zcxq98-2	Position	P1-CE	Instrument Name	Instrument 1	User Name	
Inj Vol	0.1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	zcxq98-2.d	ACQ Method	SIBU-ESI-1.m	Comment		Acquired Time	11/2/2016 3:12:56 PM



**Figure 11S.** Negative ESI-MS spectrum of compound **2c**

Data File: E:\DATA\2017\0802\ZQ-254-2.lcd

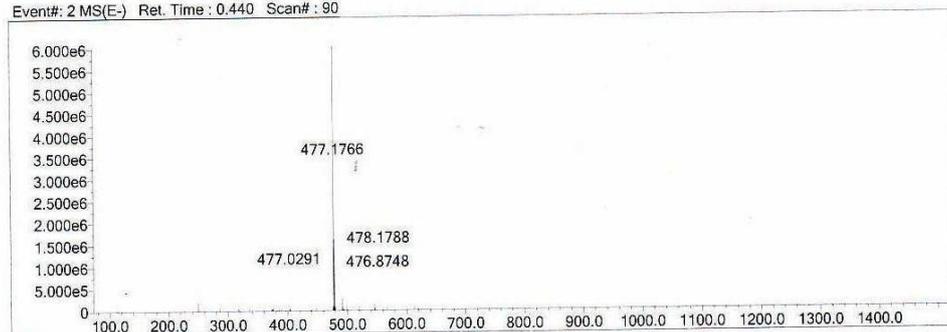
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B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	10	Mg	2	0	0	Br	1	0	0					

Error Margin (ppm): 10  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

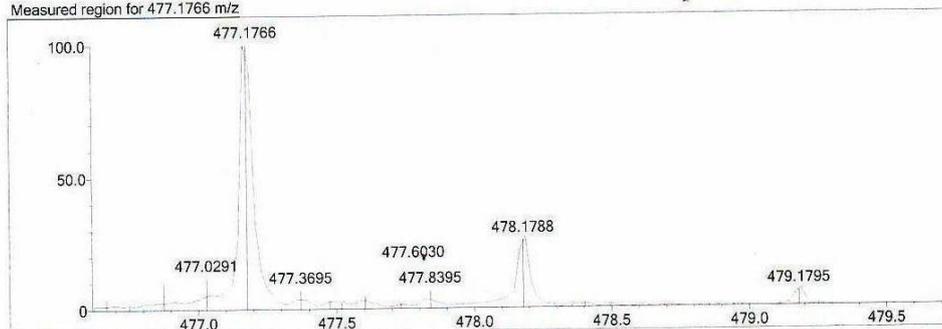
DBE Range: -2.0 - 100.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

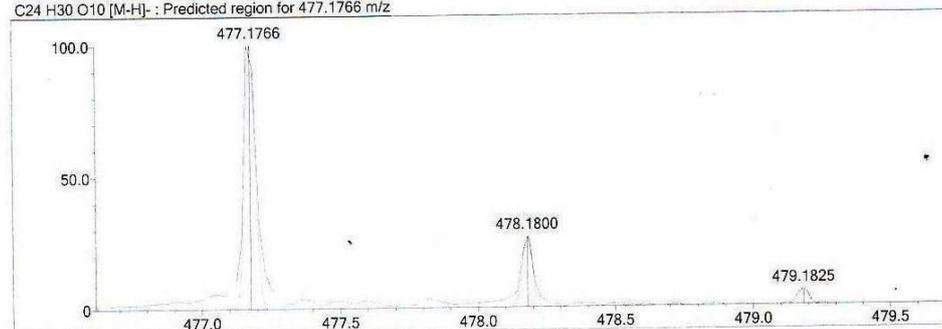
Event#: 2 MS(E-) Ret. Time : 0.440 Scan# : 90



Measured region for 477.1766 m/z

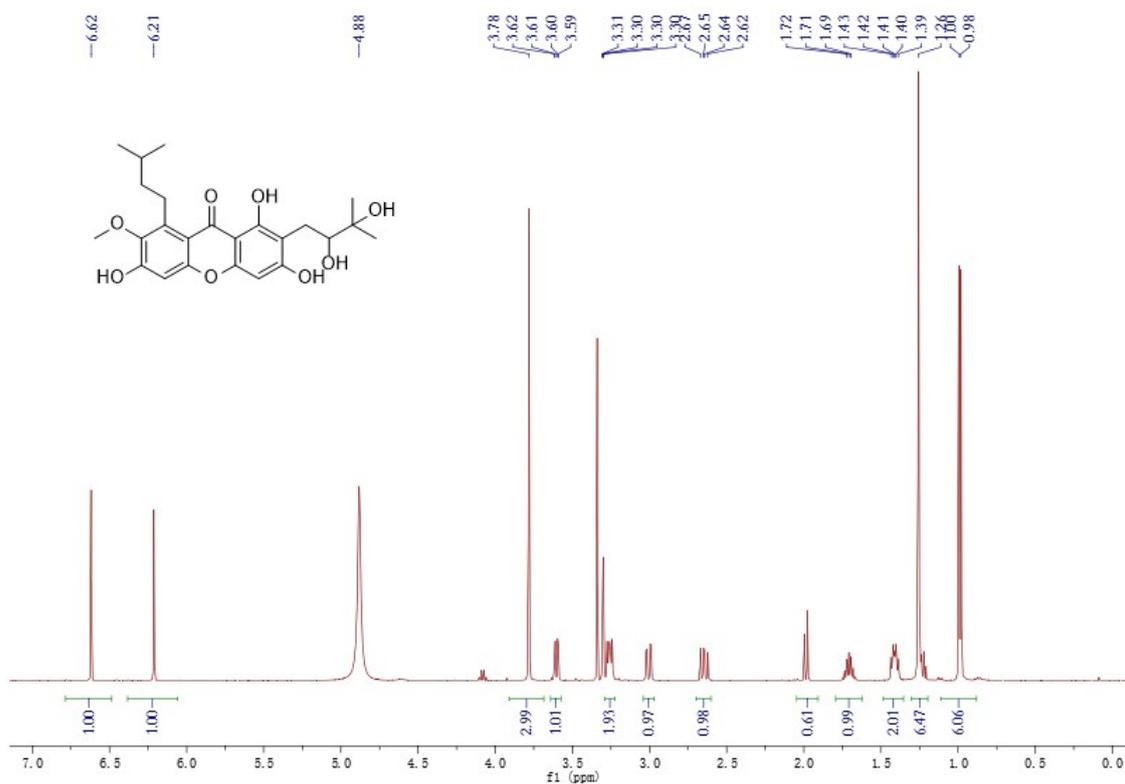


C24 H30 O10 [M-H]- : Predicted region for 477.1766 m/z

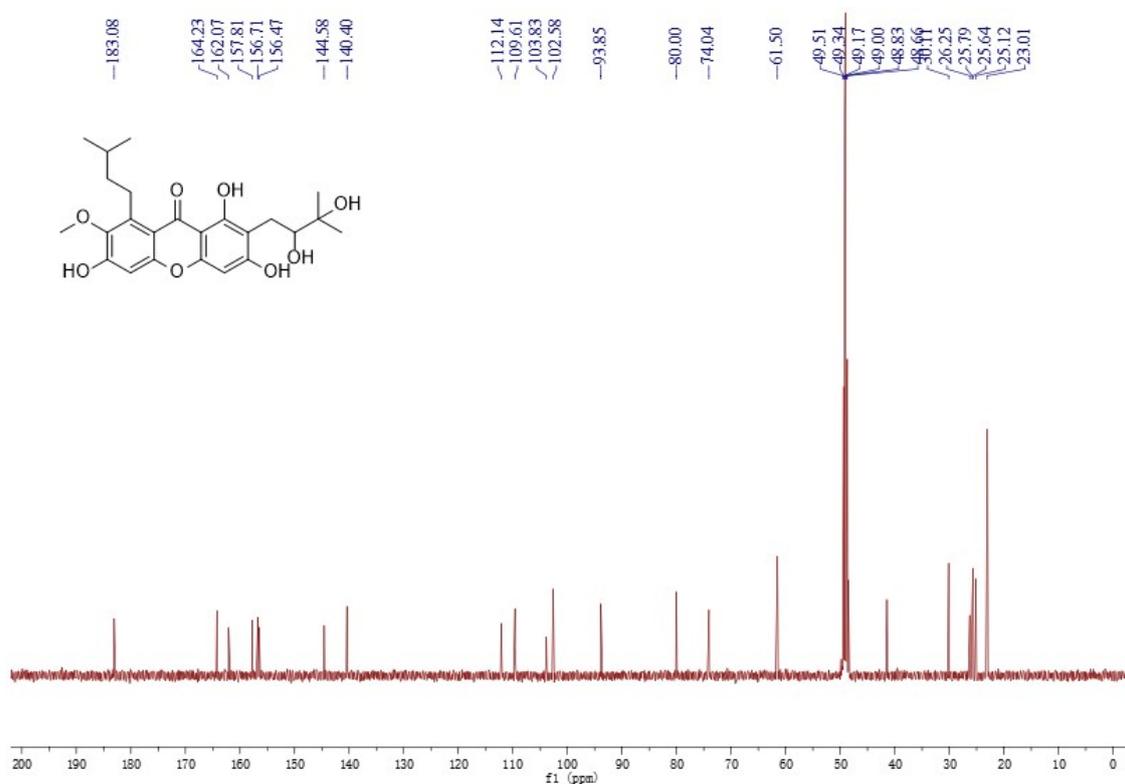


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C24 H30 O10	[M-H]-	477.1766	477.1766	-0.0	0.00	10.0

Figure 12S. Negative HR-ESIMS spectrum of compound 2c

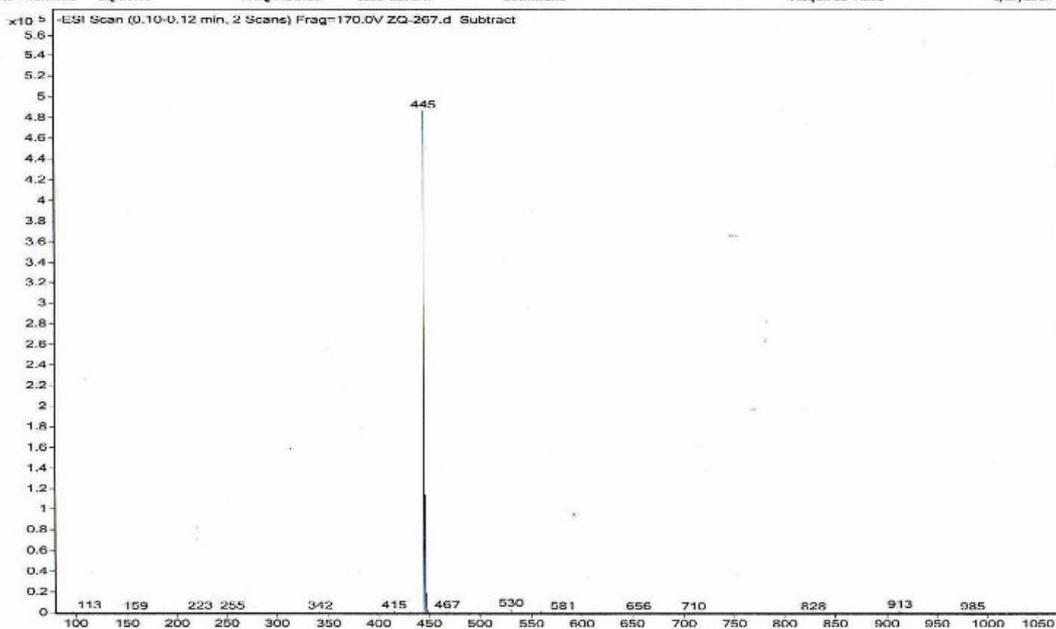


**Figure 13S.** <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 500 MHz) of compound 2d



**Figure 14S.** <sup>13</sup>C NMR spectrum (CD<sub>3</sub>OD, 125 MHz) of compound 2d

Sample Name	ZQ-267	Position	P1-C3	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ZQ-267.d	ACQ Method	SIBU-ESI-1.m	Comment		Acquired Time	6/27/2017 12:49:30 PM



**Figure 15S.** Negative ESI-MS spectrum of compound **2d**

Data File: E:\DATA\2017\0802\ZQ-267.lcd

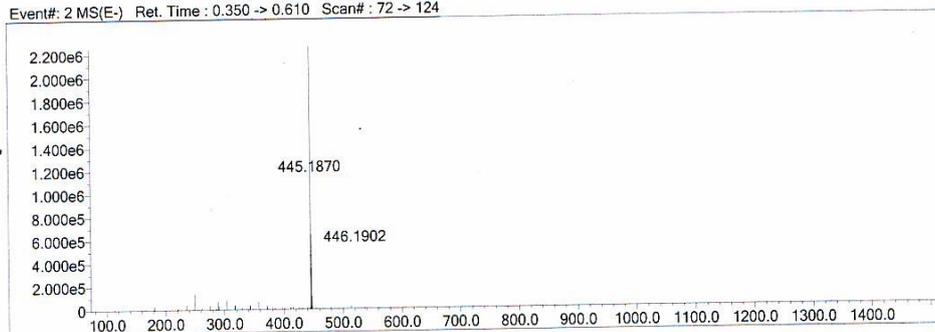
Elmt	Val.	Min	Max	Use Adduct												
H	1	0	150	O	2	0	50	S	2	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	10	Mg	2	0	0	Br	1	0	0					

Error Margin (ppm): 10  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

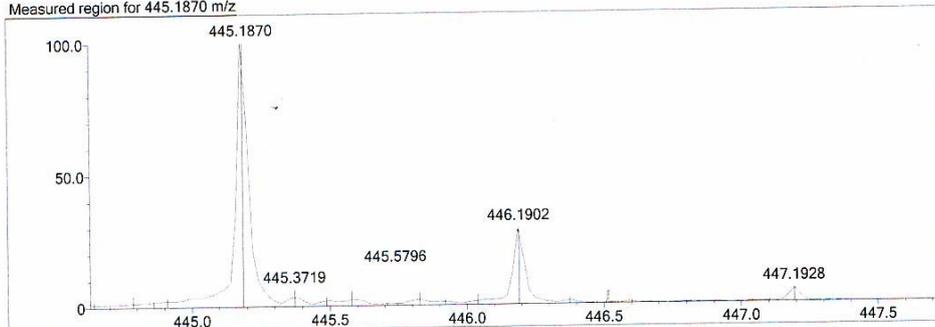
DBE Range: -2.0 - 100.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

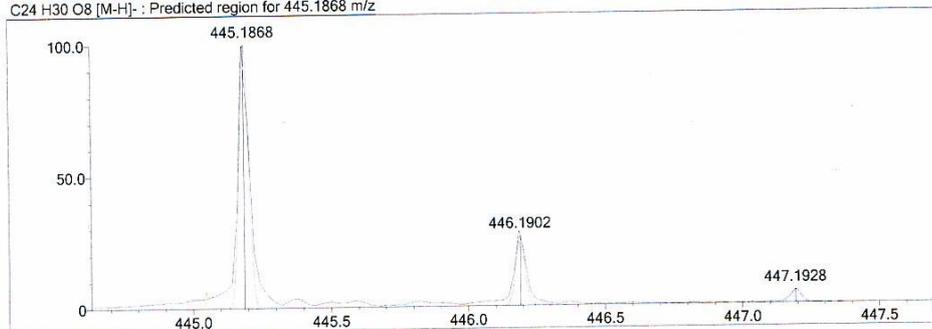
Event#: 2 MS(E-) Ret. Time : 0.350 -> 0.610 Scan# : 72 -> 124



Measured region for 445.1870 m/z



C24 H30 O8 [M-H]- : Predicted region for 445.1868 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C24 H30 O8	[M-H]-	445.1870	445.1868	0.2	0.45	10.0

Figure 16S. Negative HR-ESIMS spectrum of compound 2d

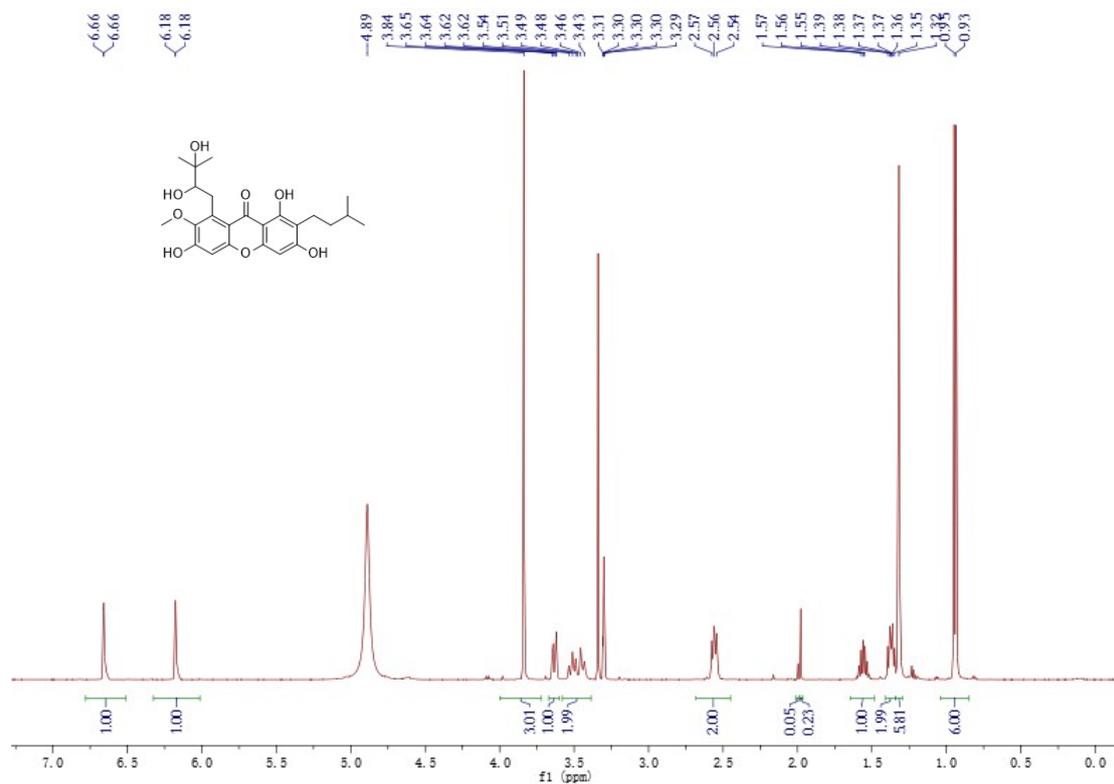


Figure 17S. <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 500 MHz) of compound 2e

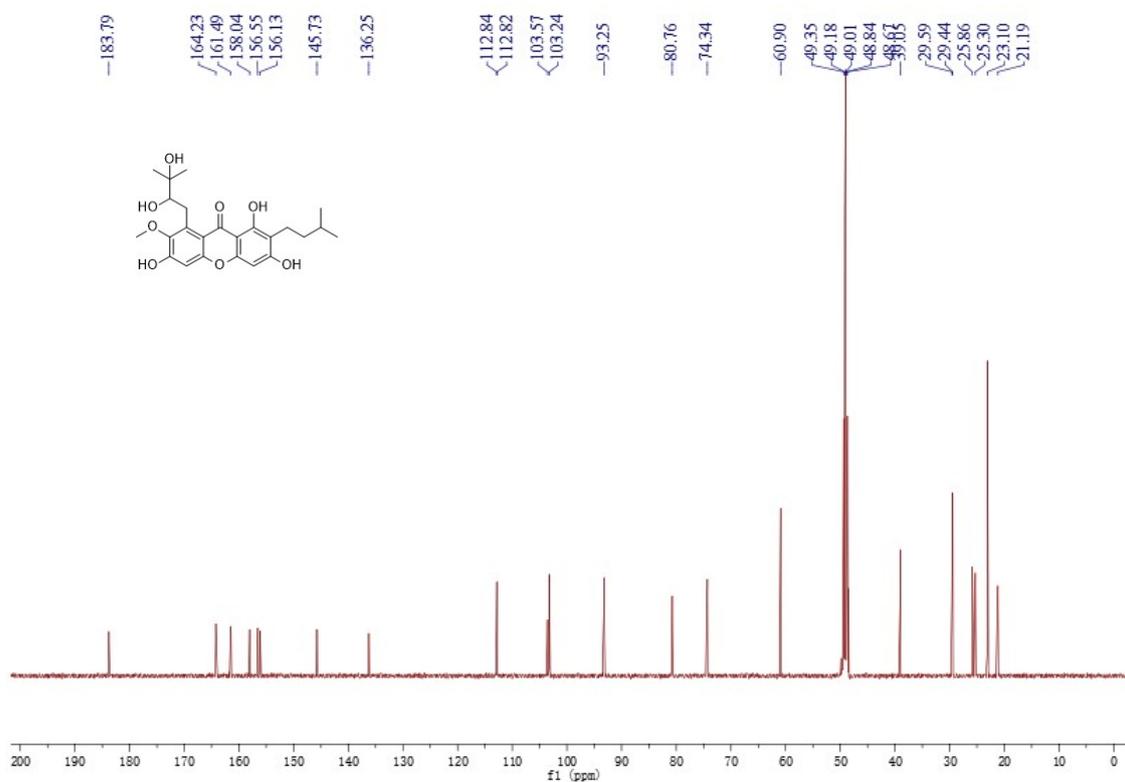
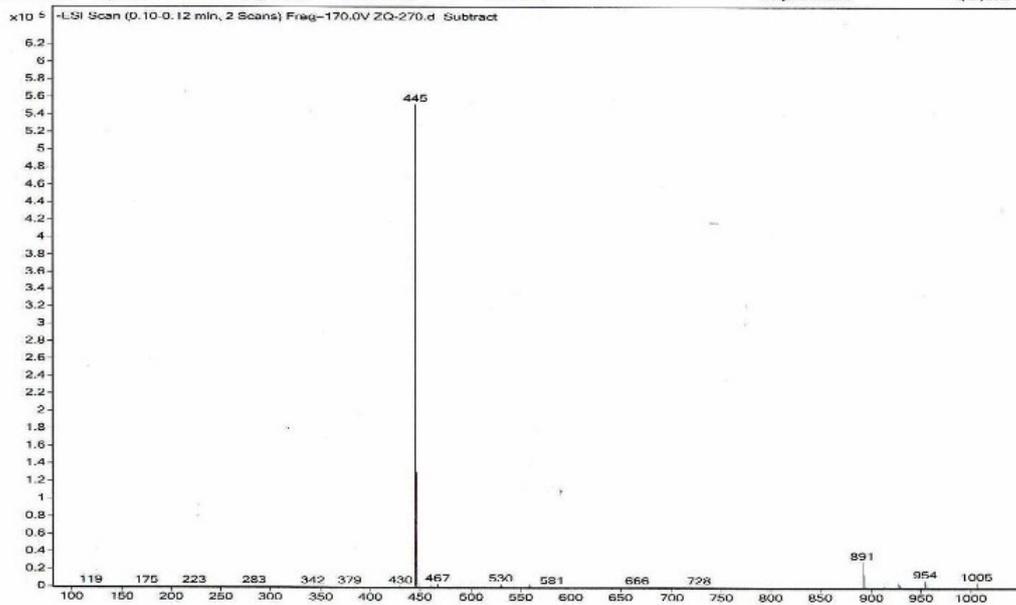


Figure 18S. <sup>13</sup>C NMR spectrum (CD<sub>3</sub>OD, 125 MHz) of compound 2e

Sample Name	ZQ-270	Position	P1-C4	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ZQ-270.d	ACQ Method	SIBU-ESI-m	Comment		Acquired Time	6/27/2017 12:50:42 PM



**Figure 19S.** Negative ESI-MS spectrum of compound **2e**

Data File: E:\DATA\2017\0802\ZQ-270.lcd

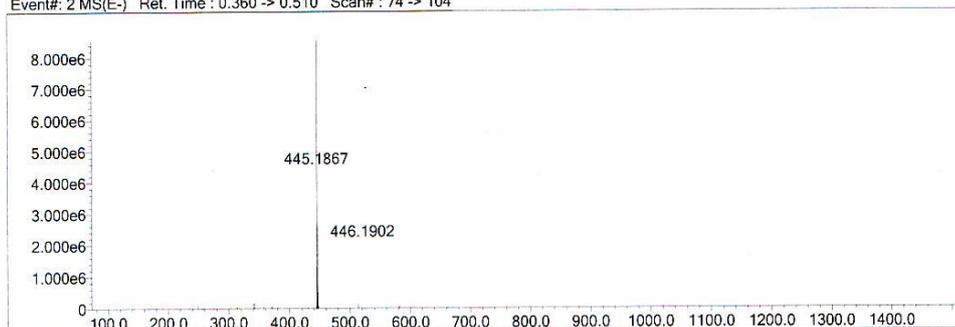
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B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	10	Mg	2	0	0	Br	1	0	0					

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 Max Isotopes: all  
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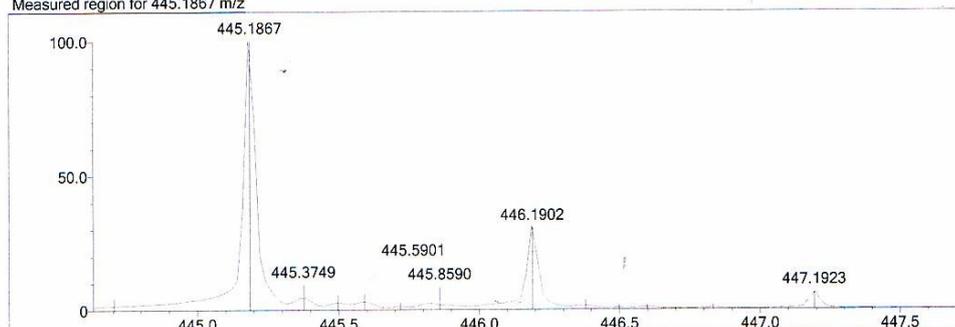
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 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
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 Max Results: 10

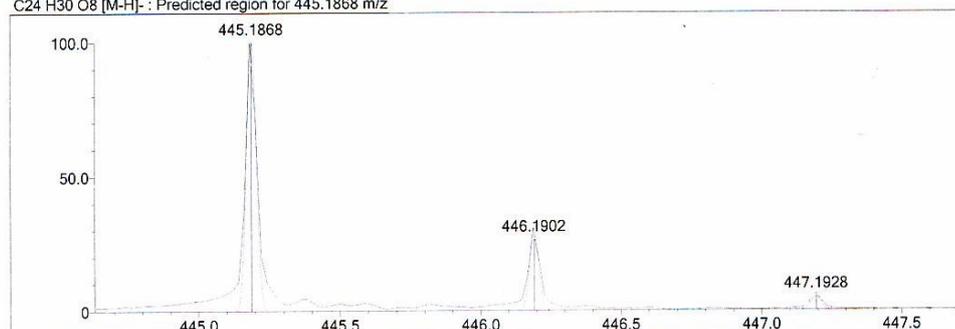
Event#: 2 MS(E-) Ret. Time : 0.360 -> 0.510 Scan# : 74 -> 104



Measured region for 445.1867 m/z

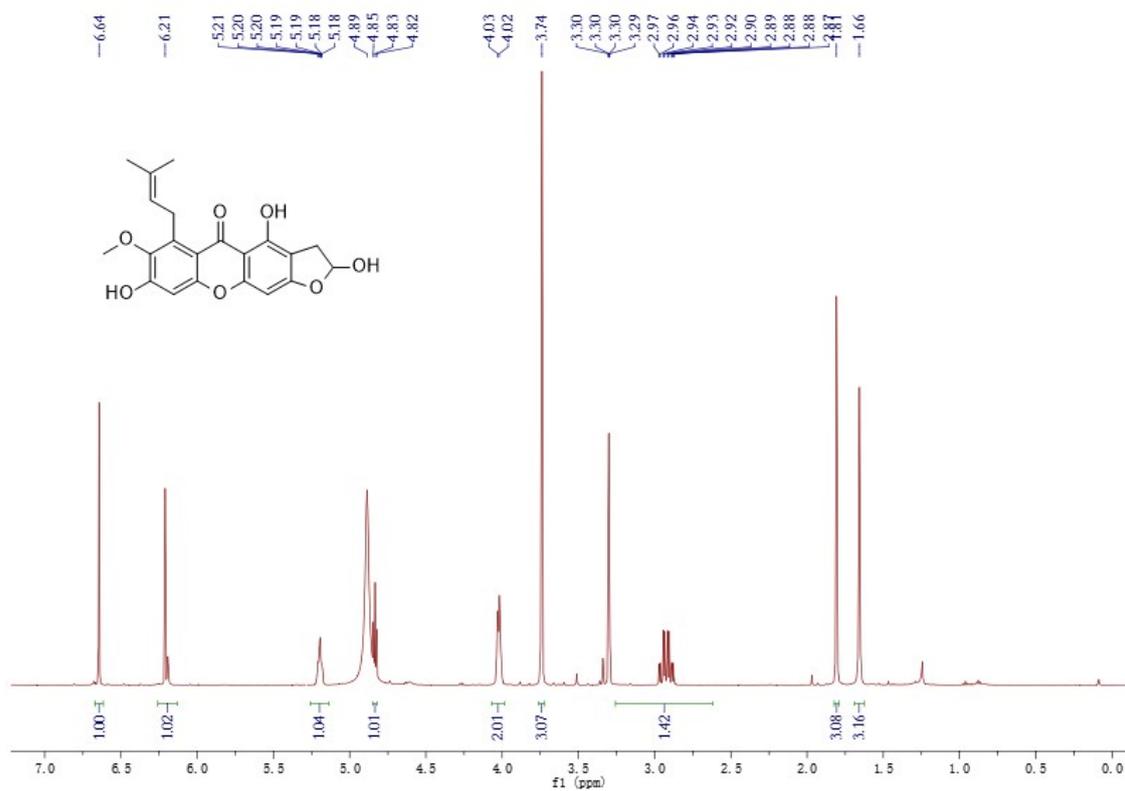


C24 H30 O8 [M-H]- : Predicted region for 445.1868 m/z

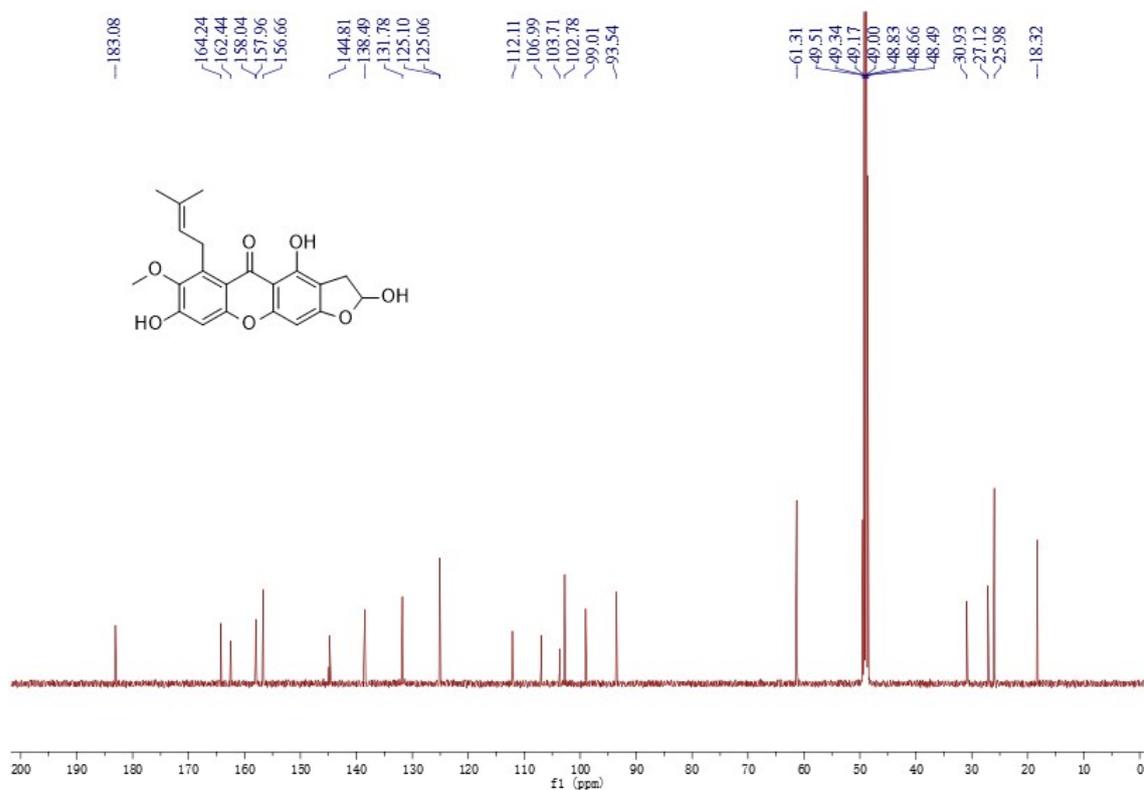


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C24 H30 O8	[M-H]-	445.1867	445.1868	-0.1	-0.22	10.0

Figure 20S. Negative HR-ESIMS spectrum of compound 2e

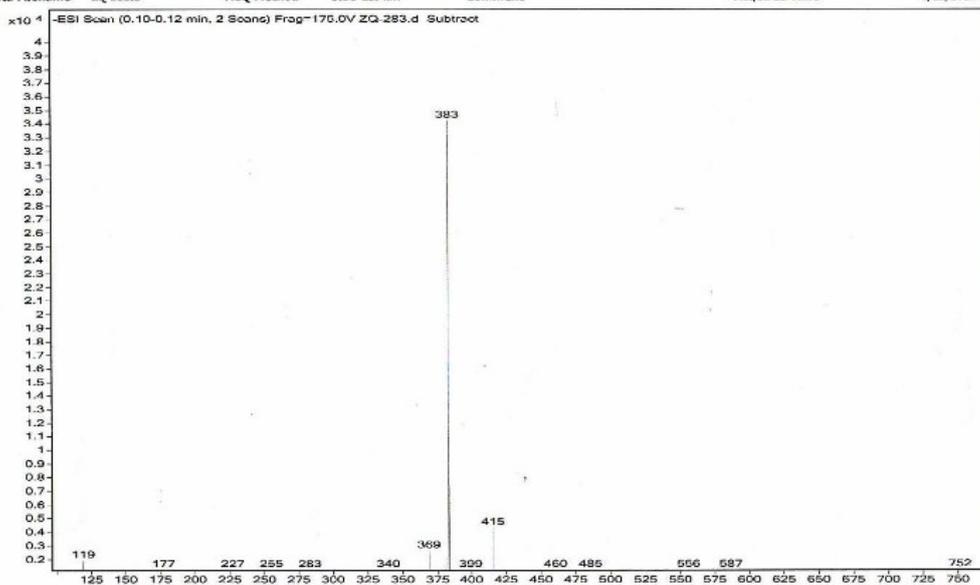


**Figure 21S.**  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 500 MHz) of compound **2f**



**Figure 22S.**  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 125 MHz) of compound **2f**

Sample Name	ZQ-283	Position	P1-B6	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ZQ-283.d	ACQ Method	SIBU-ESI-I.m	Comment		Acquired Time	7/13/2017 1:10:13 PM



**Figure 23S.** Negative ESI-MS spectrum of compound **2f**

Data File: E:\DATA\2017\0802\ZQ-283.lcd

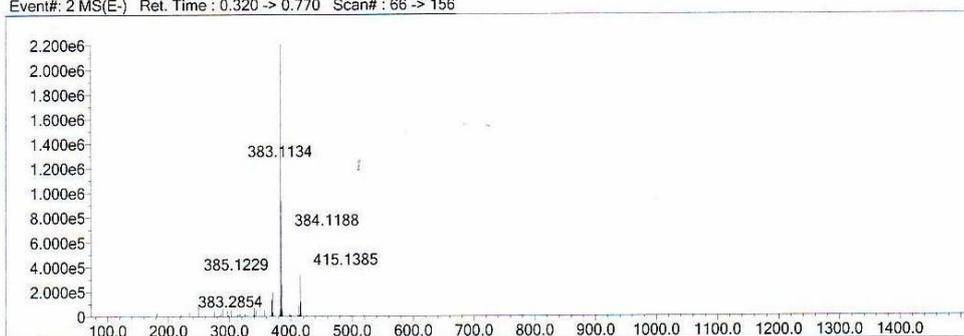
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B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	0	Mg	2	0	0	Br	1	0	5					

Error Margin (ppm): 10  
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 Max Isotopes: all  
 MSn Iso RI (%): 75.00

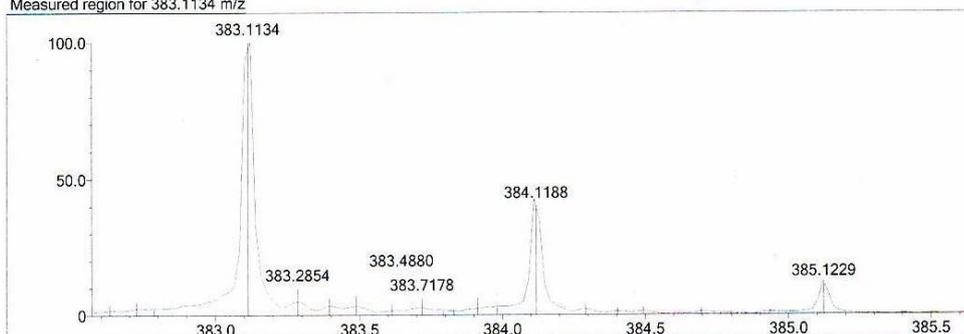
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Electron Ions: both  
 Use MSn Info: yes  
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 Max Results: 10

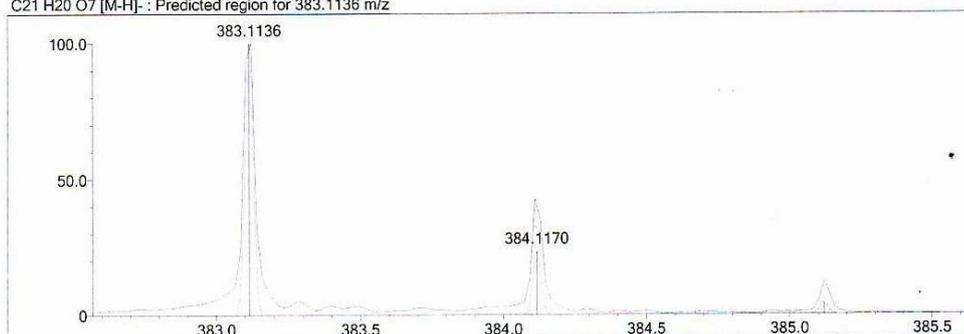
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Measured region for 383.1134 m/z

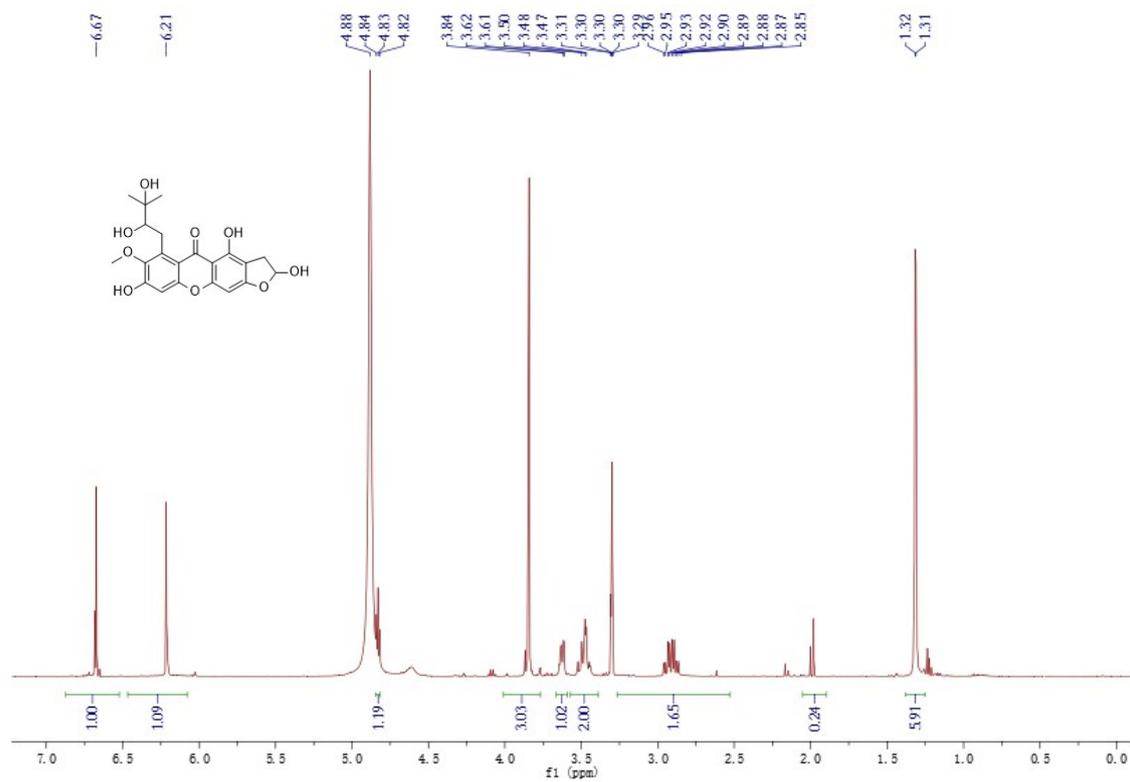


C21 H20 O7 [M-H]- : Predicted region for 383.1136 m/z

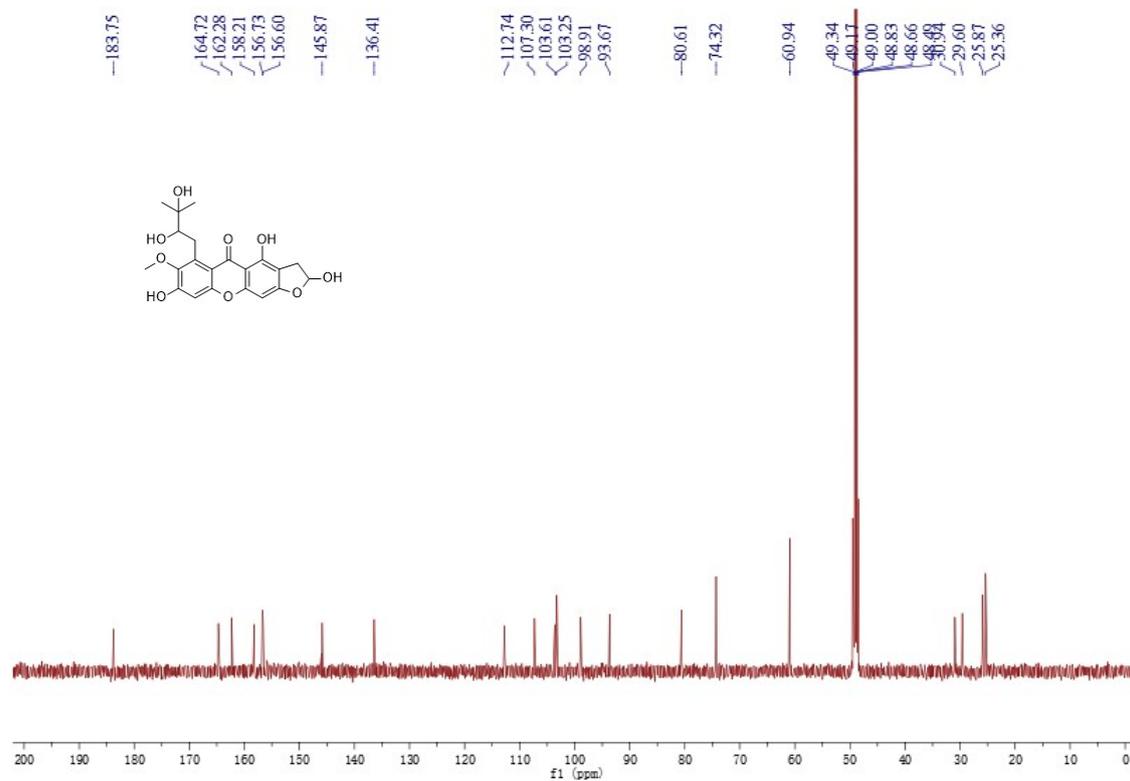


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C21 H20 O7	[M-H]-	383.1134	383.1136	-0.2	-0.52	12.0

Figure 24S. Negative HR-ESIMS spectrum of compound 2f

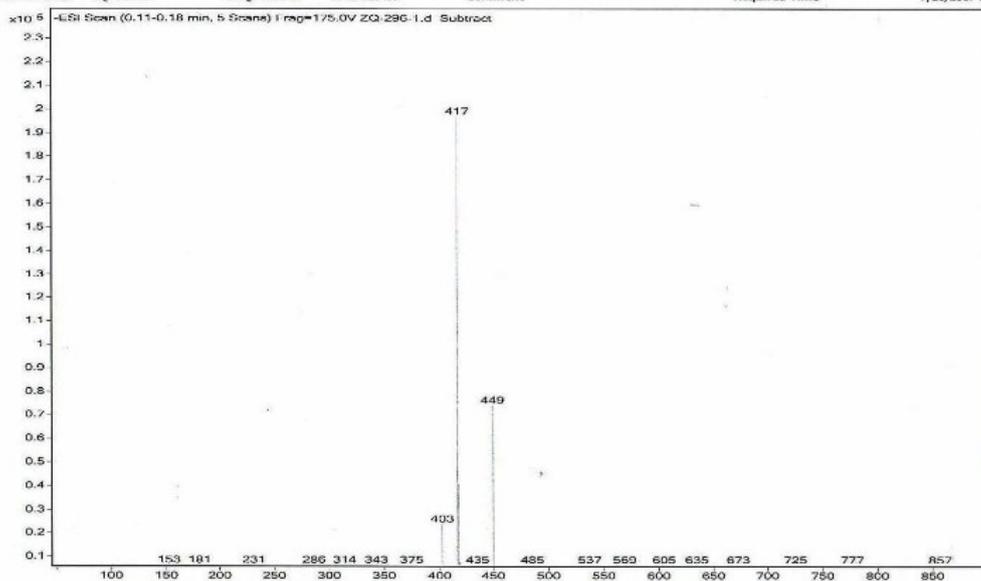


**Figure 25S.**  $^1\text{H}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 500 MHz) of compound **2g**



**Figure 26S.**  $^{13}\text{C}$  NMR spectrum ( $\text{CD}_3\text{OD}$ , 125 MHz) of compound **2g**

Sample Name	ZQ-296-1	Position	P1-D1	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ZQ-296-1.d	ACQ Method	SIBU-ESI-LM	Comment		Acquired Time	7/20/2017 9:24:13 AM



**Figure 27S.** Negative ESI-MS spectrum of compound **2g**

Data File: E:\DATA\2017\0802\ZQ-296-1.lcd

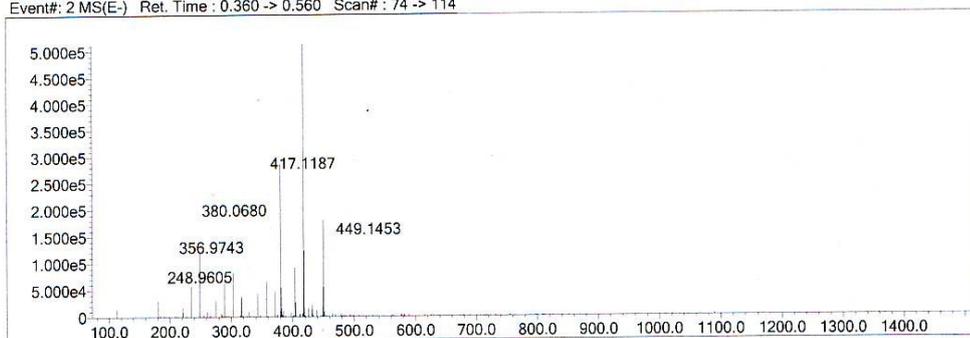
Elmt	Val.	Min	Max	Use Adduct												
H	1	0	150	O	2	0	50	S	2	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	0	Mg	2	0	0	Br	1	0	5					

Error Margin (ppm): 10  
 HC Ratio: unlimited  
 \* Max Isotopes: all  
 MSn Iso RI (%): 75.00

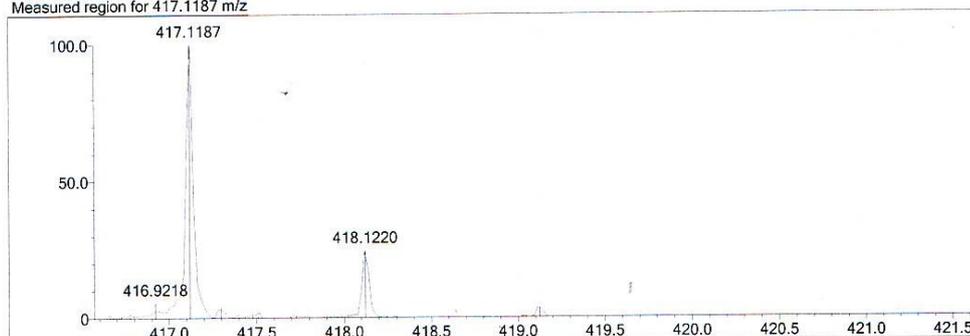
DBE Range: -2.0 - 100.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

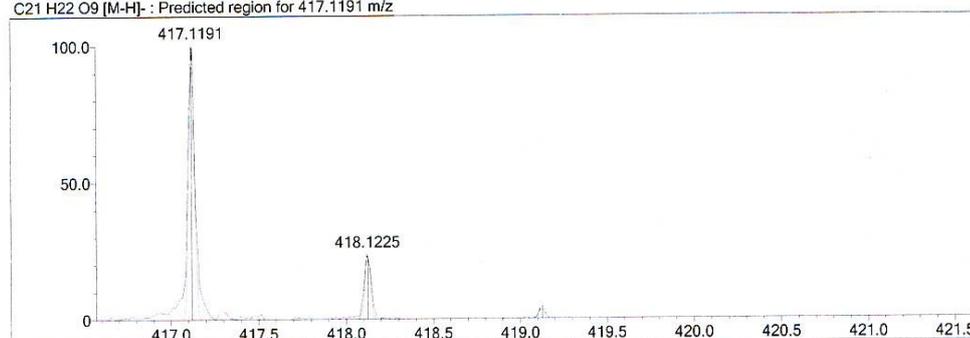
Event#: 2 MS(E-) Ret. Time : 0.360 -> 0.560 Scan# : 74 -> 114



Measured region for 417.1187 m/z

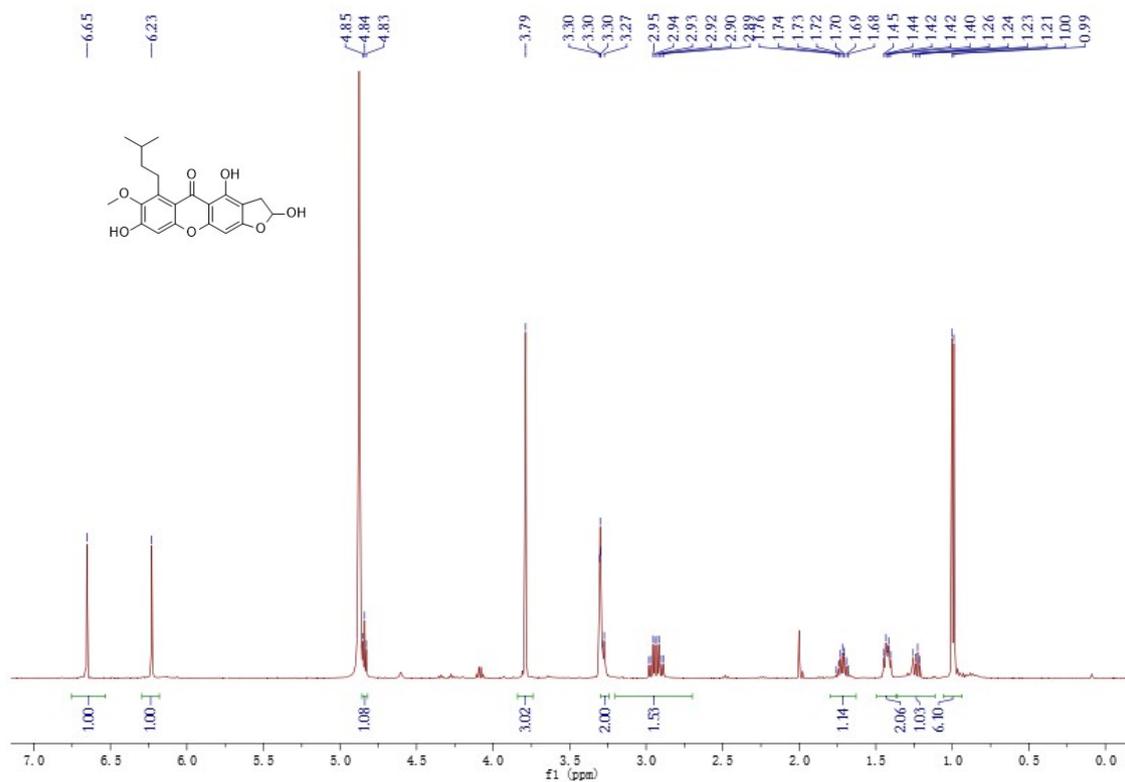


C21 H22 O9 [M-H]- : Predicted region for 417.1191 m/z

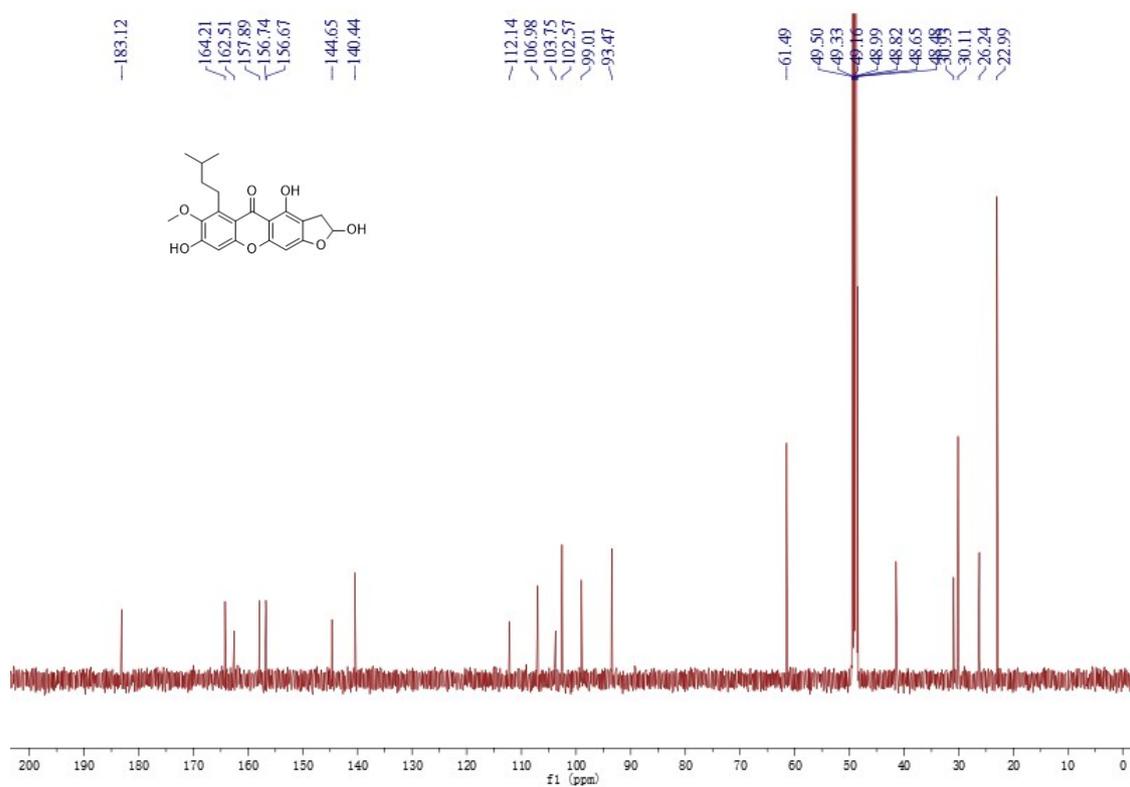


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C21 H22 O9	[M-H]-	417.1187	417.1191	-0.4	-0.96	11.0

Figure 28S. Negative HR-ESIMS spectrum of compound 2g



**Figure 29S.** <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 500 MHz) of compound 2h



**Figure 30S.** <sup>13</sup>C NMR spectrum (CD<sub>3</sub>OD, 125 MHz) of compound 2h

==== LCMSsolution Data Report ====

Acquired by : Admin  
Date Acquired : 2017/8/14 19:06:40  
Sample Name : ZQ-316  
Data File : ZQ-316.lcd  
Method File : 阻尼管一級20151028-100-1500.lcm

System Configuration  
<<Instrument>> : LC-IT-TOF

<Spectrum>

Retention Time: 0.440 (Scan#: 91)  
Spectrum: Averaged 0.350-0.540 (72-110)  
Background: Averaged 0.000-0.333 (2-68) MS Stage: MS Polarity: Neg Segment1 - Event2 Precursor: ---- Cutoff:

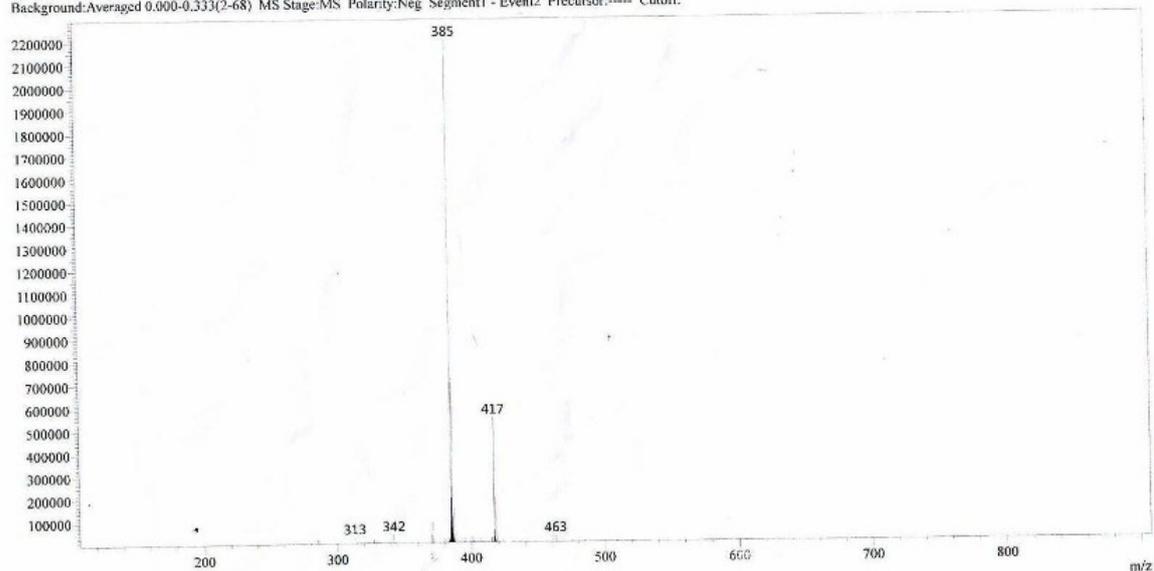


Figure 31S. Negative ESI-MS spectrum of compound 2h

Data File: E:\DATA\2017\0816\ZQ-316.lcd

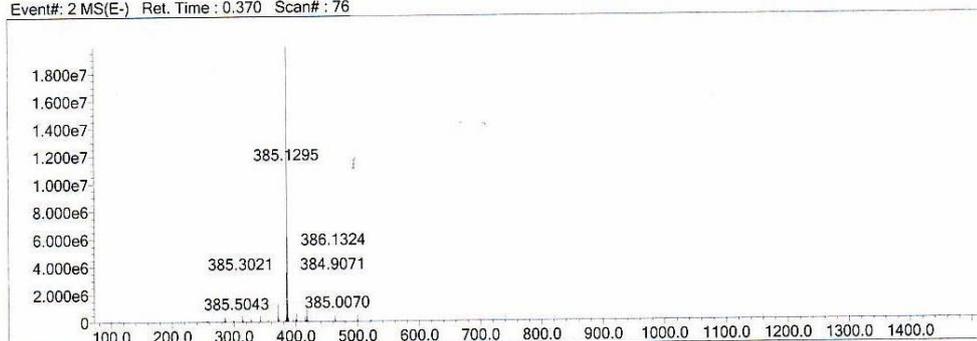
Elmt	Val.	Min	Max	Use Adduct												
H	1	0	150	O	2	0	50	P	3	0	0	Br	1	0	0	H
B	3	0	0	F	1	0	0	S	2	0	0	I	3	0	0	
C	4	0	100	Na	1	0	0	Cl	1	0	0	Pt	2	0	0	
N	3	0	0	Mg	2	0	0	Fe	2	0	0					

Error Margin (ppm): 10  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

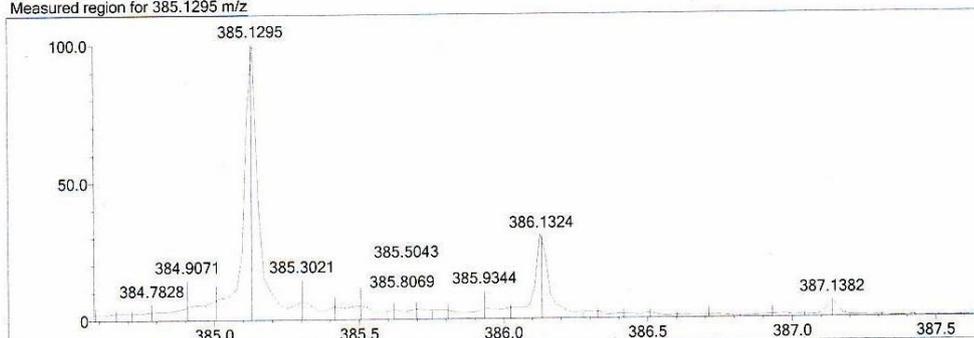
DBE Range: -2.0 - 100.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

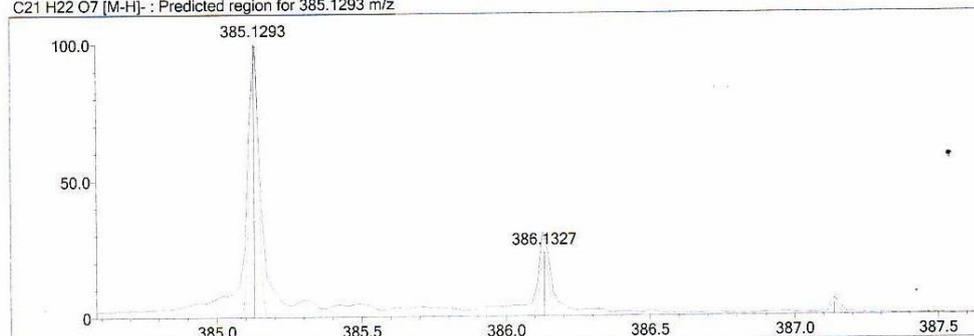
Event#: 2 MS(E-) Ret. Time : 0.370 Scan# : 76



Measured region for 385.1295 m/z

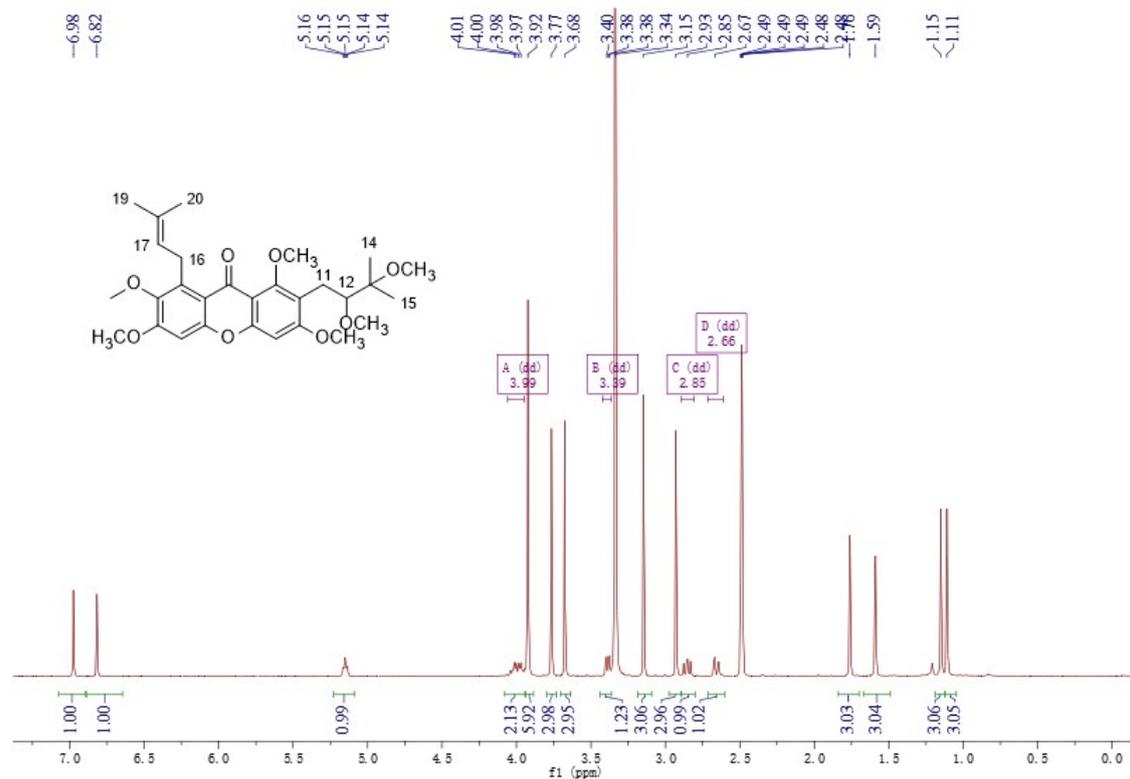


C21 H22 O7 [M-H]- : Predicted region for 385.1293 m/z

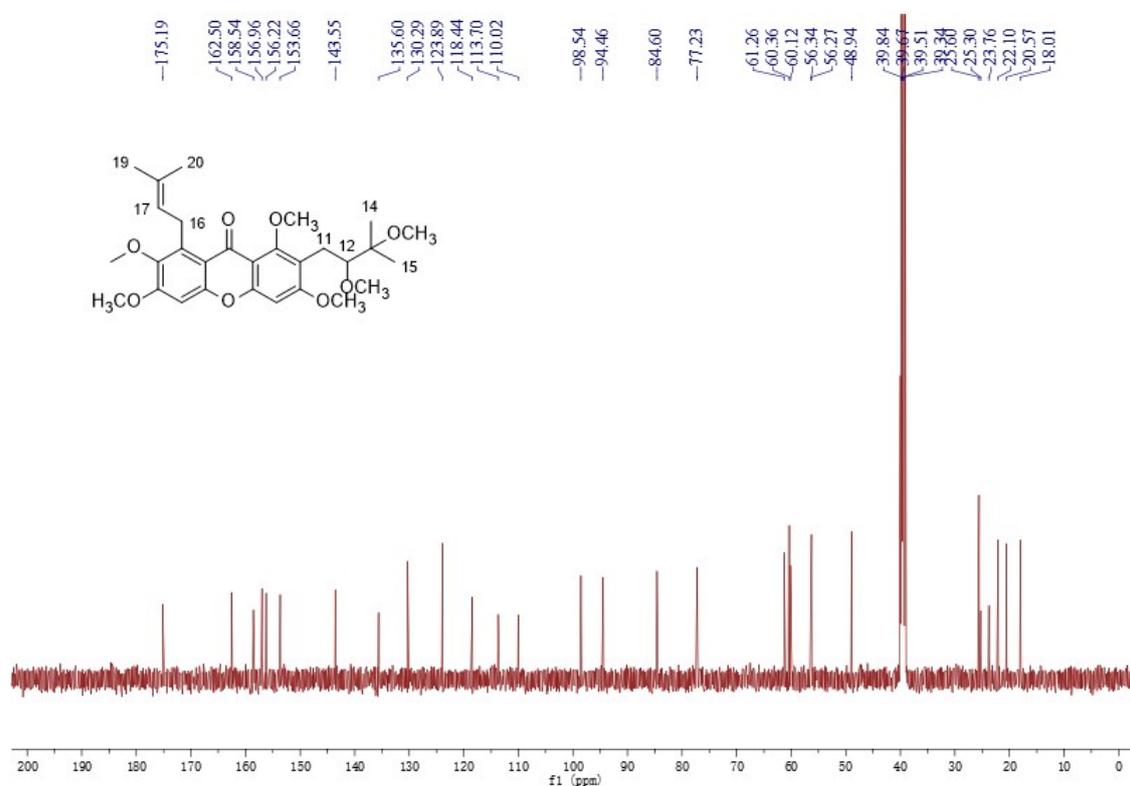


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C21 H22 O7	[M-H]-	385.1295	385.1293	0.2	0.52	11.0

Figure 32S. Negative HR-ESIMS spectrum of compound 2h



**Figure 33S.** <sup>1</sup>H NMR spectrum (DMSO-*d*<sub>6</sub>, 500 MHz) of compound 2i



**Figure 34S.** <sup>13</sup>C NMR spectrum (DMSO-*d*<sub>6</sub>, 125 MHz) of compound 2i

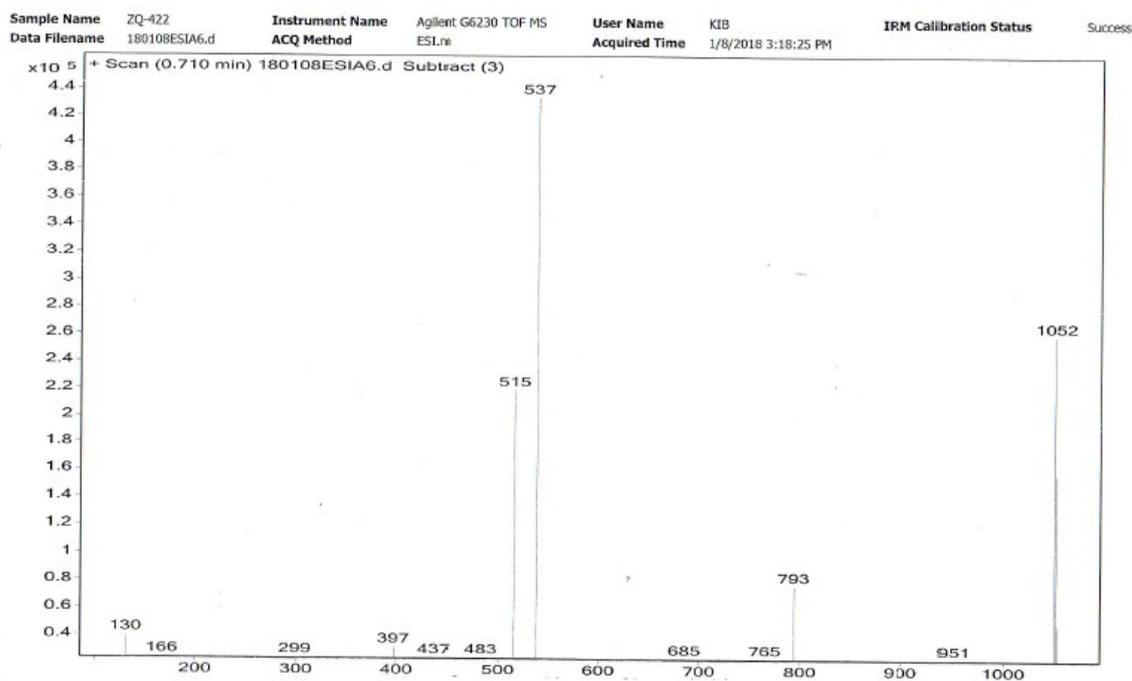


Figure 35S. Positive ESI-MS spectrum of compound 2i

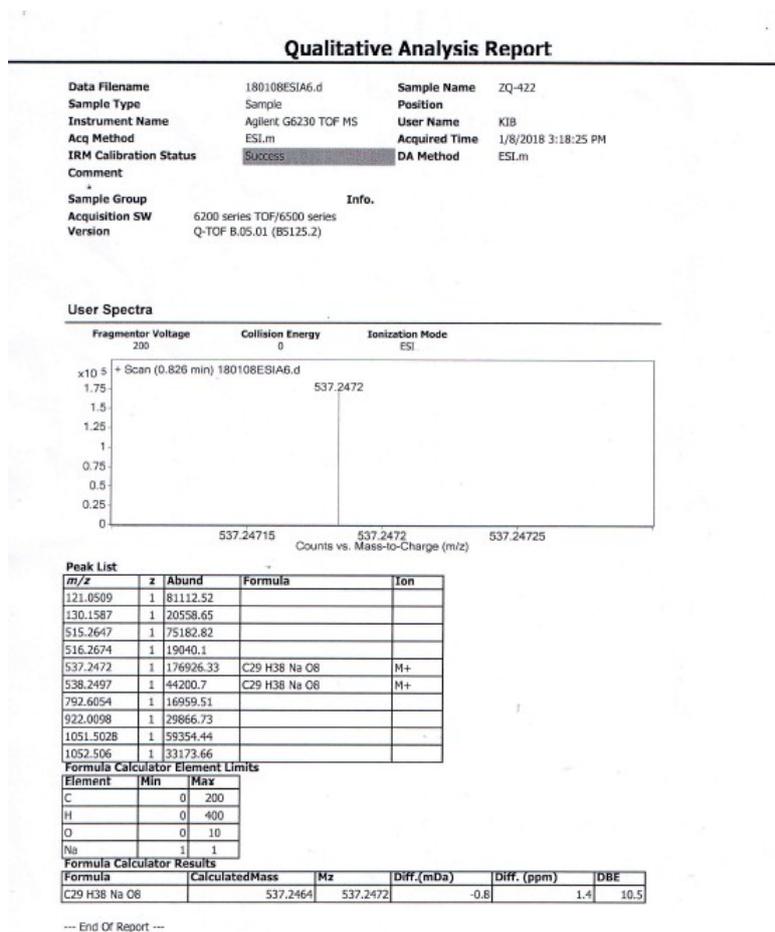
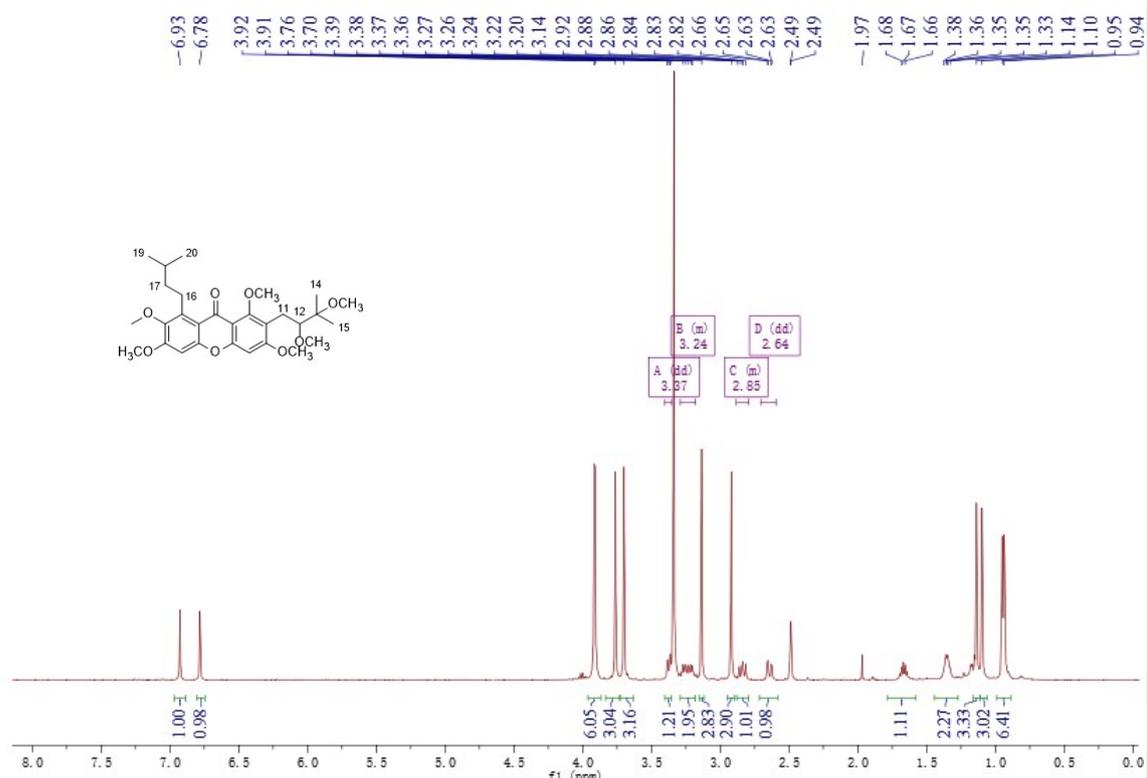
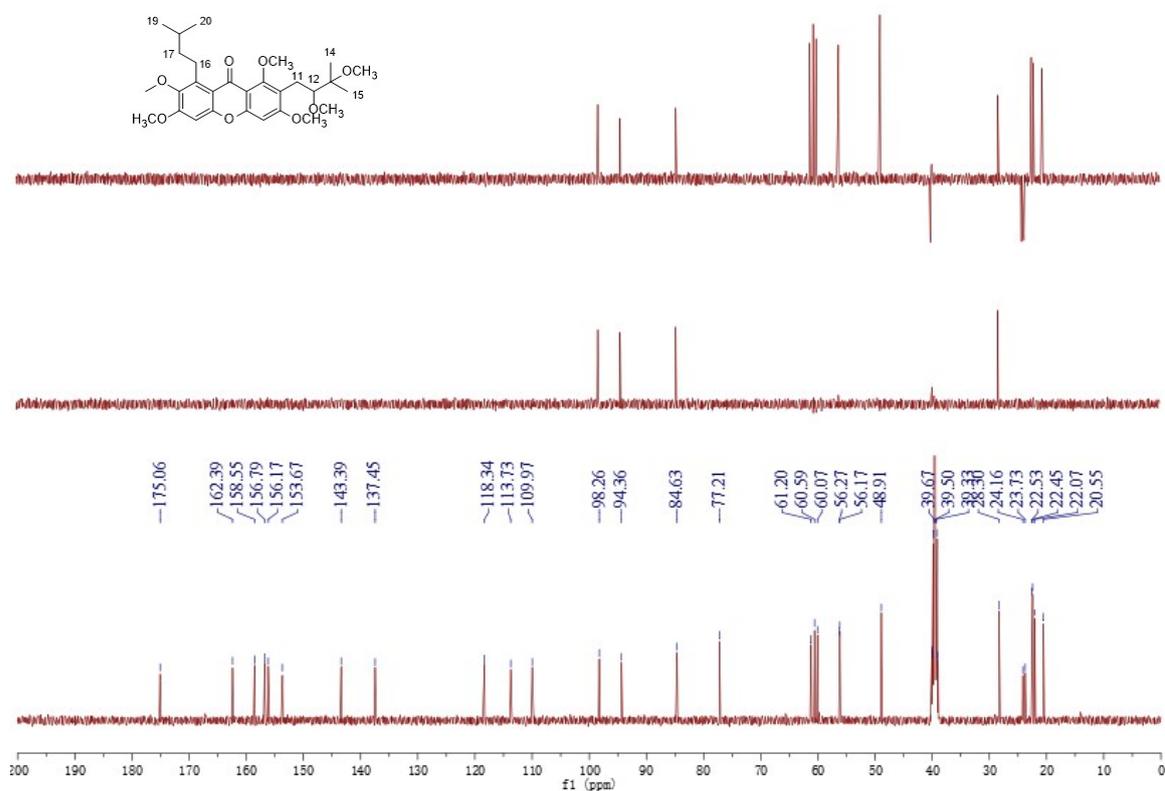


Figure 36S. Positive HR-ESIMS spectrum of compound 2i



**Figure 37S.** <sup>1</sup>H NMR spectrum (DMSO-*d*<sub>6</sub>, 500 MHz) of compound 2j



**Figure 38S.** <sup>13</sup>C NMR spectrum (DMSO-*d*<sub>6</sub>, 125 MHz) of compound 2j

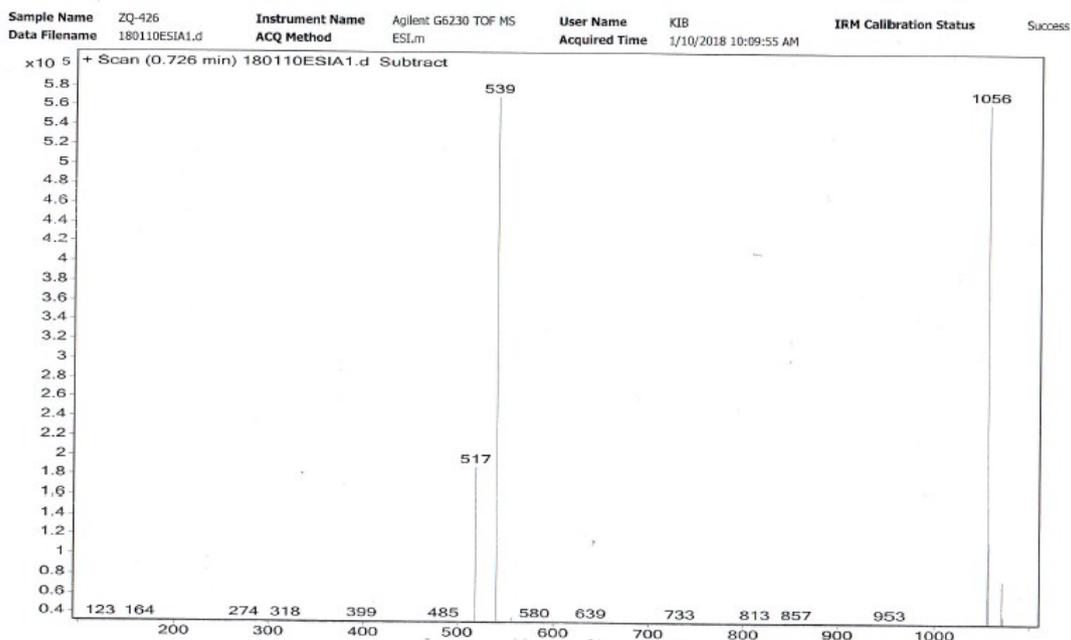


Figure 39S. Positive ESI-MS spectrum of compound 2j

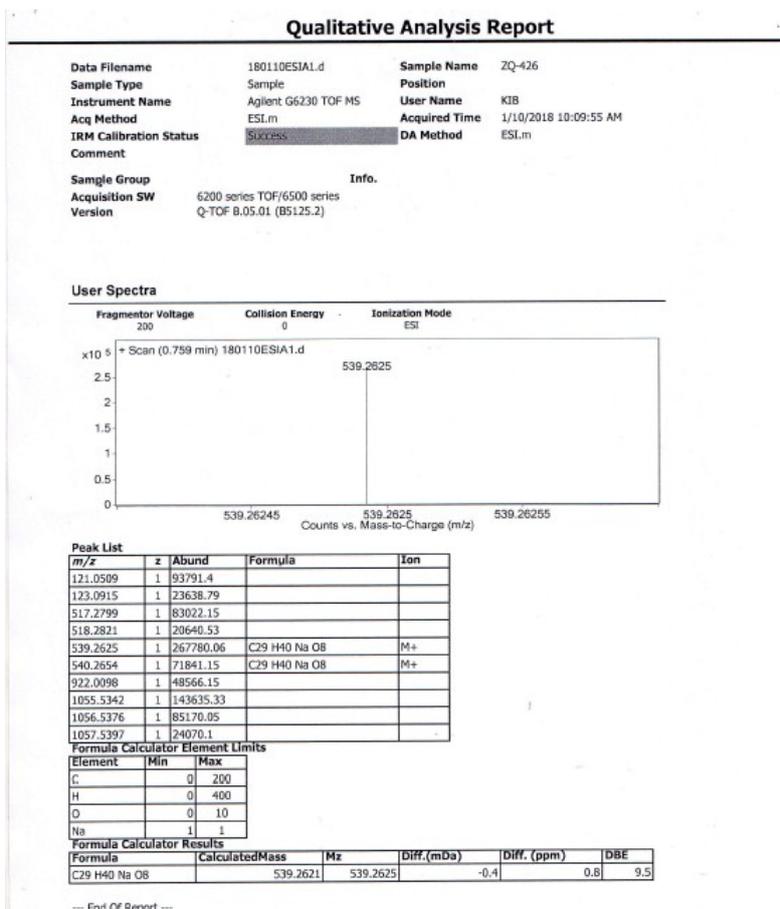


Figure 40S. Positive HR-ESIMS spectrum of compound 2j

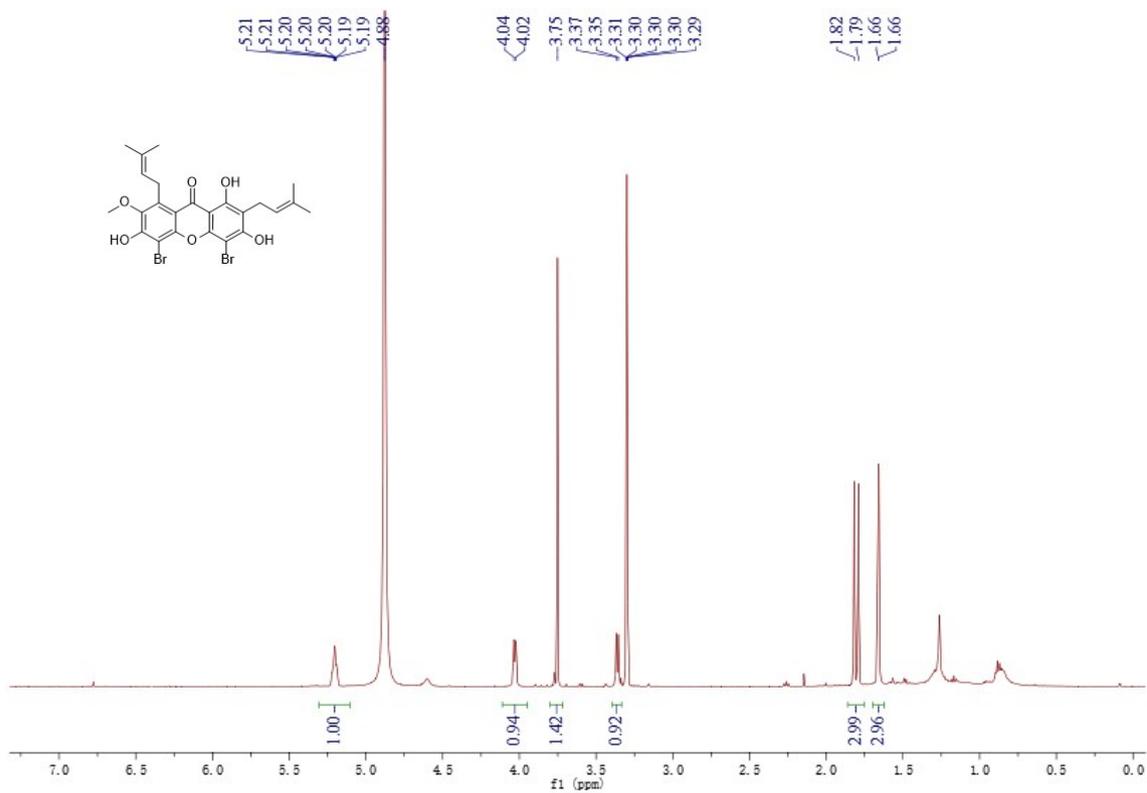


Figure 41S. <sup>1</sup>H NMR spectrum (CD<sub>3</sub>OD, 500 MHz) of compound 3c

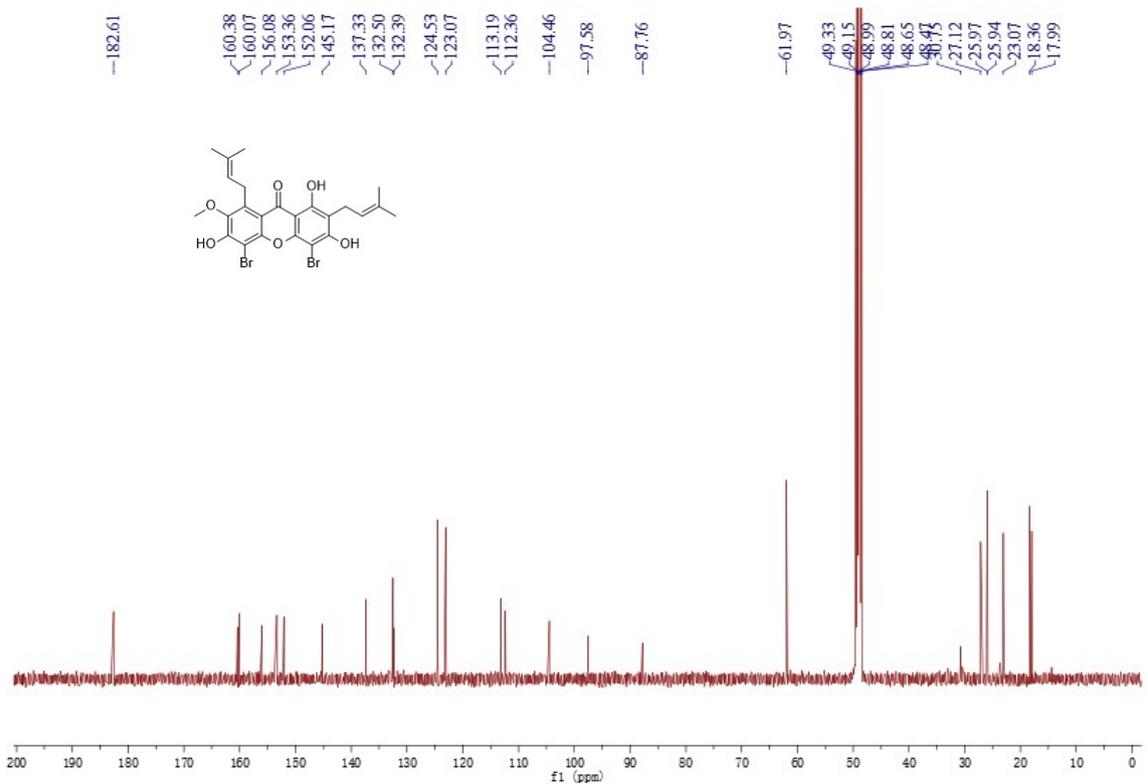


Figure 42S. <sup>13</sup>C NMR spectrum (CD<sub>3</sub>OD, 125 MHz) of compound 3c

Sample Name	ZQ-280	Position	P1-E7	Instrument Name	Instrument 1	User Name	
Inj Vol	0.3	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ZQ-280.d	ACQ Method	SIBU-ESI-Lm	Comment		Acquired Time	7/18/2017 2:15:50 PM

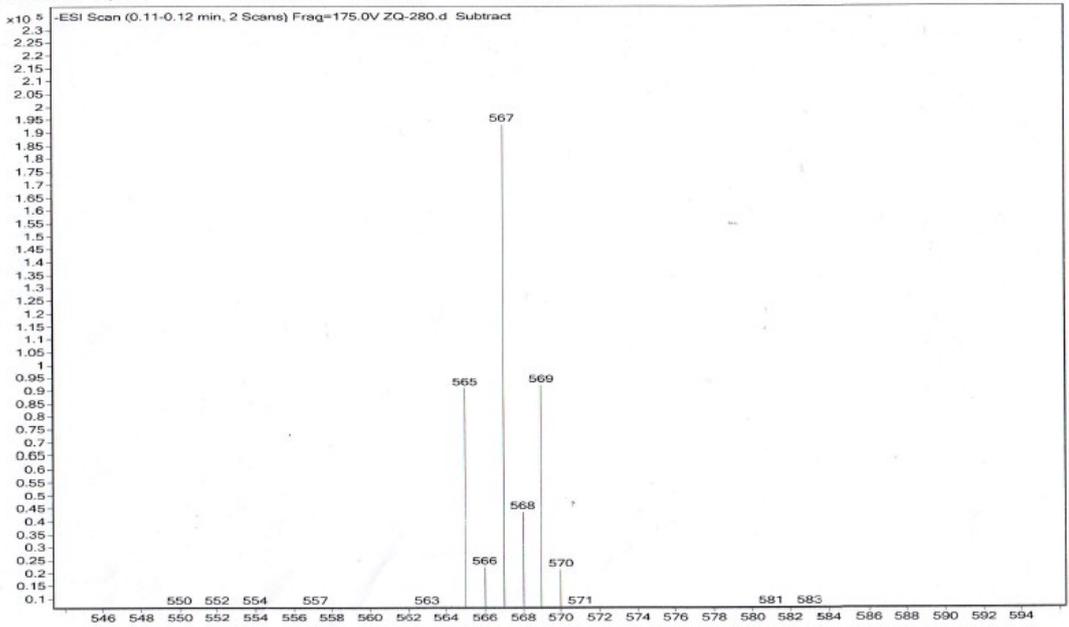


Figure 43S. Negative ESI-MS spectrum of compound 3c

Data File: E:\DATA\2017\0802\ZQ-280.Icd

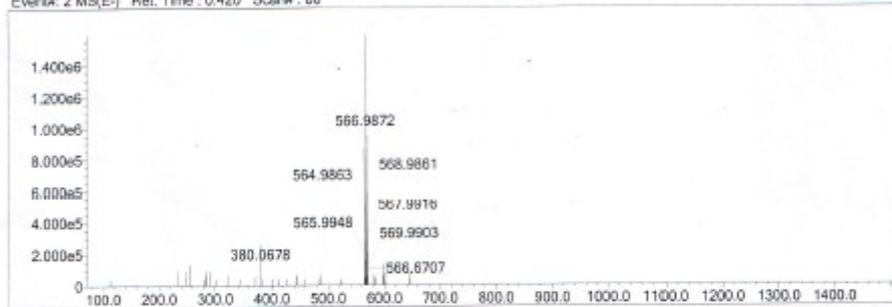
Elmt	Val.	Min	Max	Use Adduct												
H	1	0	150	O	2	0	50	S	2	0	0	I	3	0	0	H
B	3	0	0	F	1	0	0	Cl	1	0	0	Pt	2	0	0	
C	4	0	82	Na	1	0	0	Fe	2	0	0					
N	3	0	0	Mg	2	0	0	Br	1	0	5					

Engr Margin (ppm): 10  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

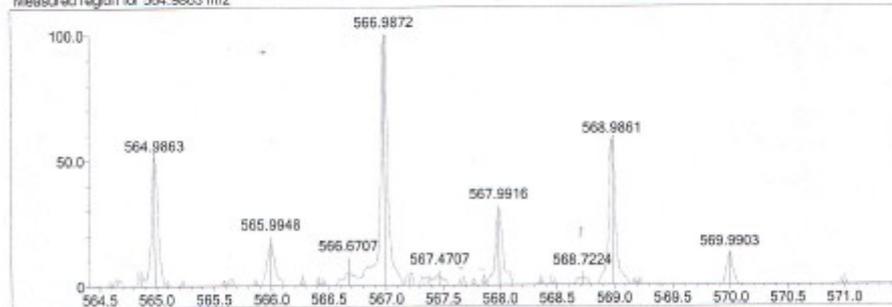
DBE Range: -2.0 - 100.0  
 Apply N Rule: yes  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

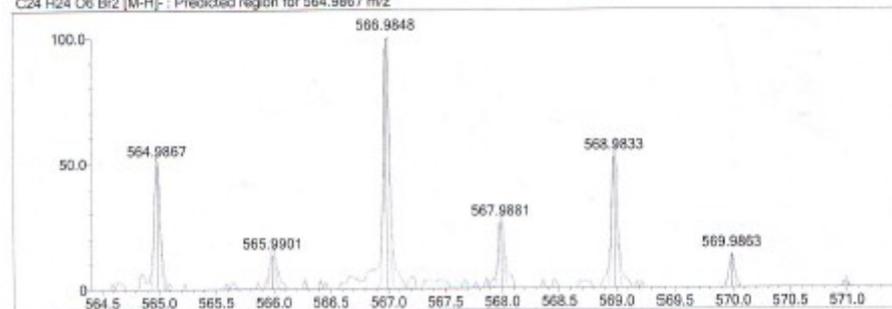
Event#: 2 MS(E-) Ret. Time : 0.420 Scan#: 86



Measured region for 564.9863 m/z

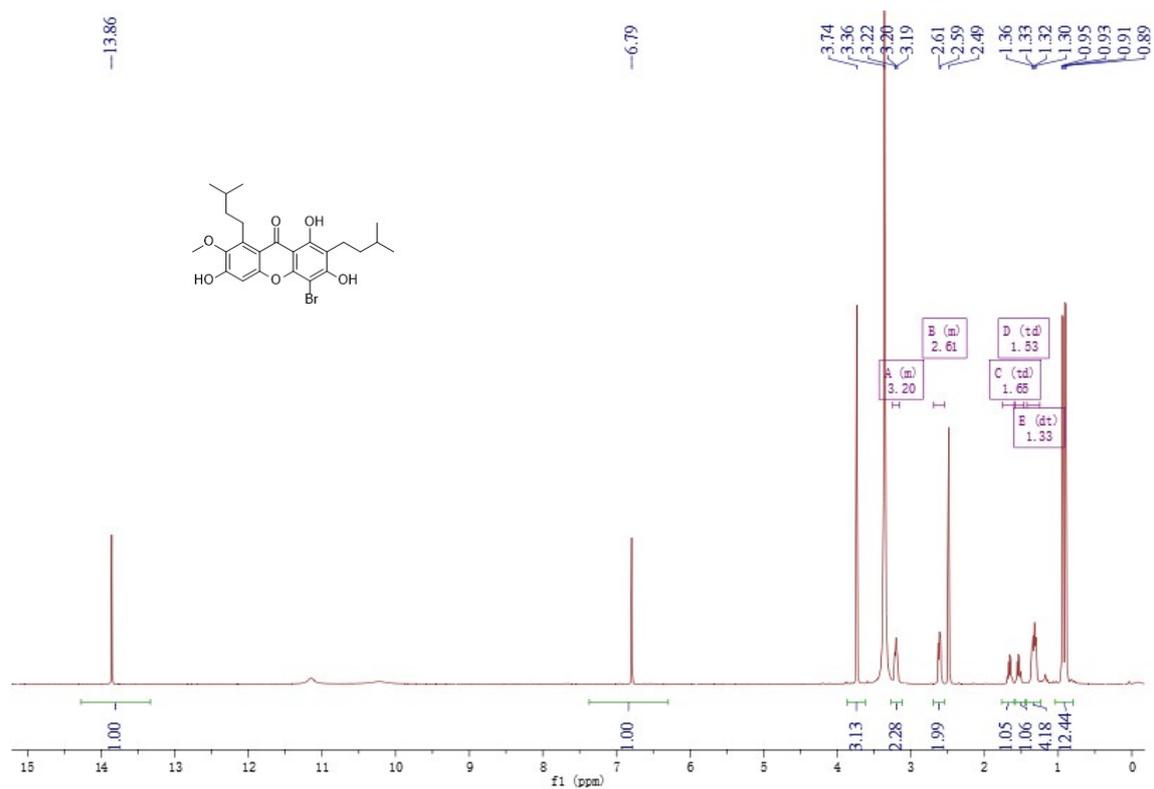


C24 H24 O6 Br2 [M-H]-: Predicted region for 564.9867 m/z

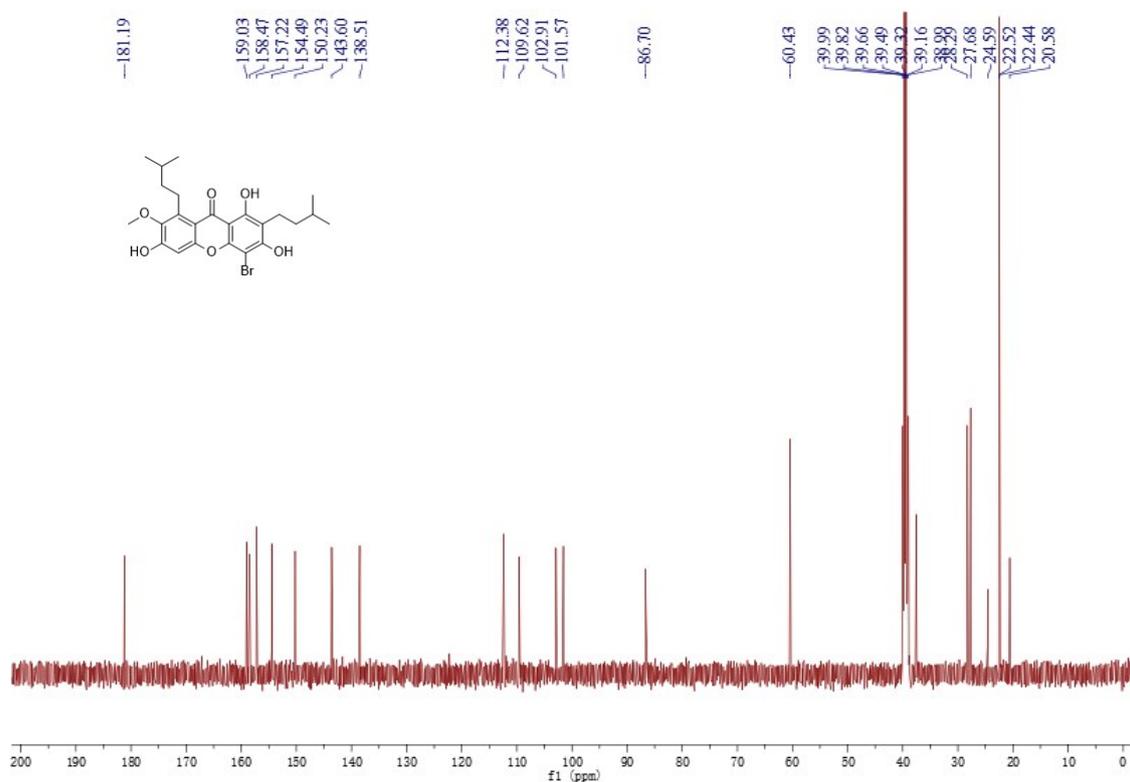


Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C24 H24 O6 Br2	[M-H]-	564.9863	564.9867	-0.4	-0.71	12.0

Figure 44S. Negative HR-ESIMS spectrum of compound 3c



**Figure 45S.** <sup>1</sup>H NMR spectrum (DMSO-*d*<sub>6</sub>, 500 MHz) of compound 3d



**Figure 46S.** <sup>13</sup>C NMR spectrum (DMSO-*d*<sub>6</sub>, 125 MHz) of compound 3d

Sample Name ZQ-369-1 Instrument Name Agilent G6230 TOF MS User Name KIB IRM Calibration Status Success  
 Data Filename 171110ESINA5.d ACQ Method ESIN.m Acquired Time 11/10/2017 11:38:10 AM

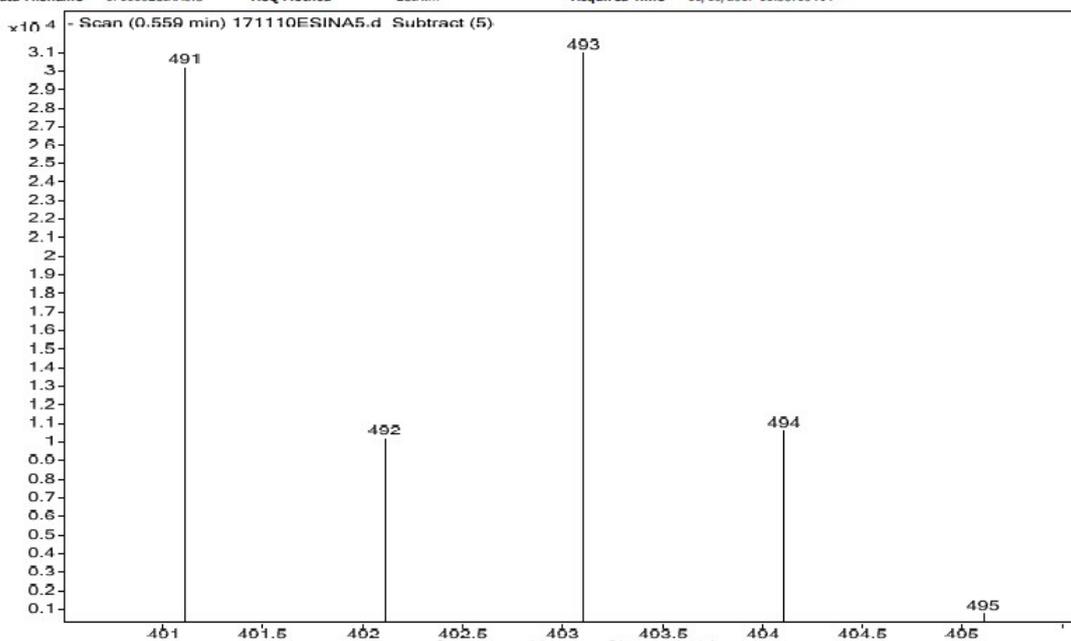


Figure 47S. Negative ESI-MS spectrum of compound 3d

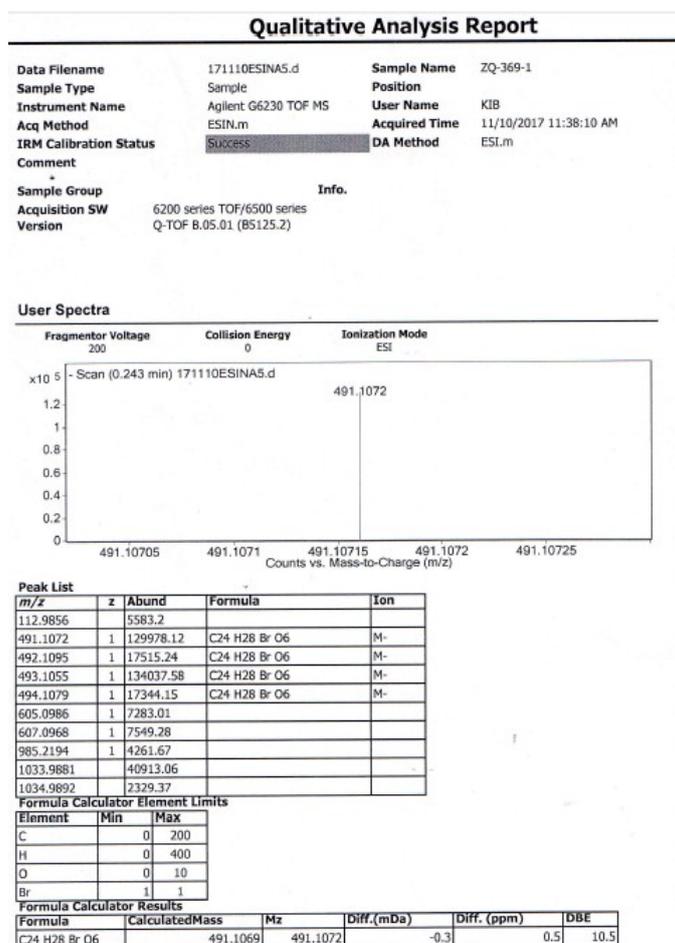
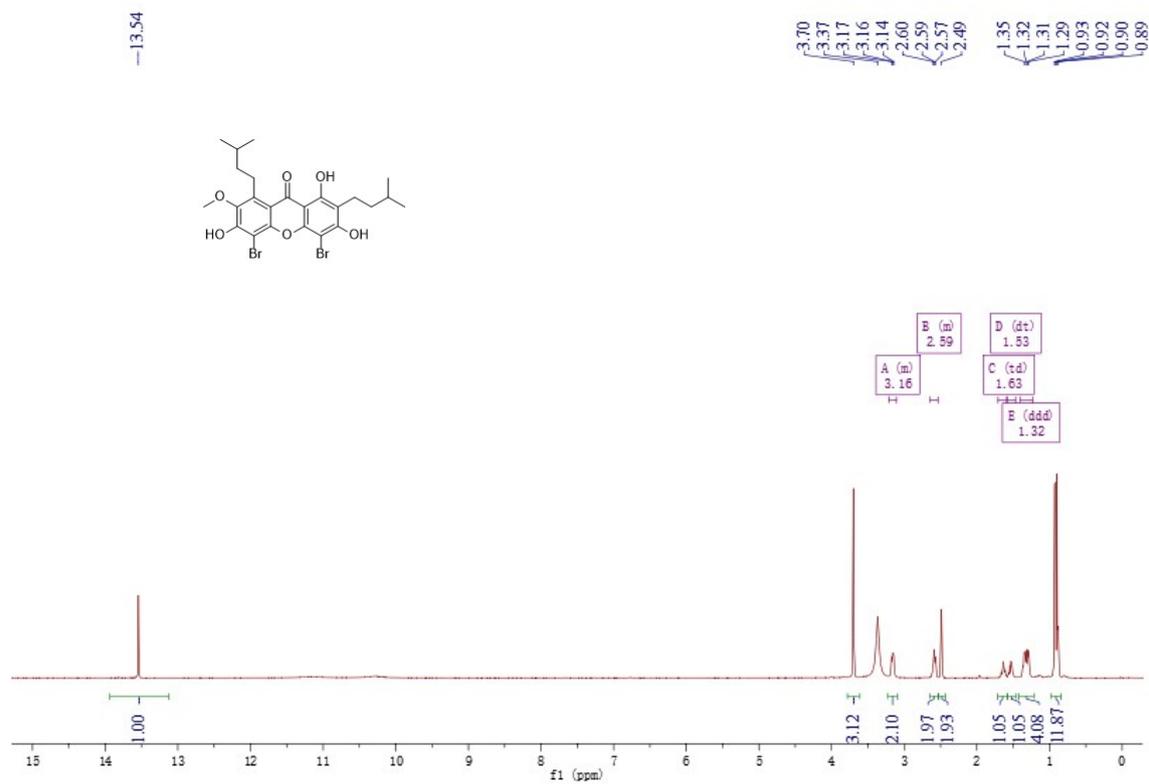
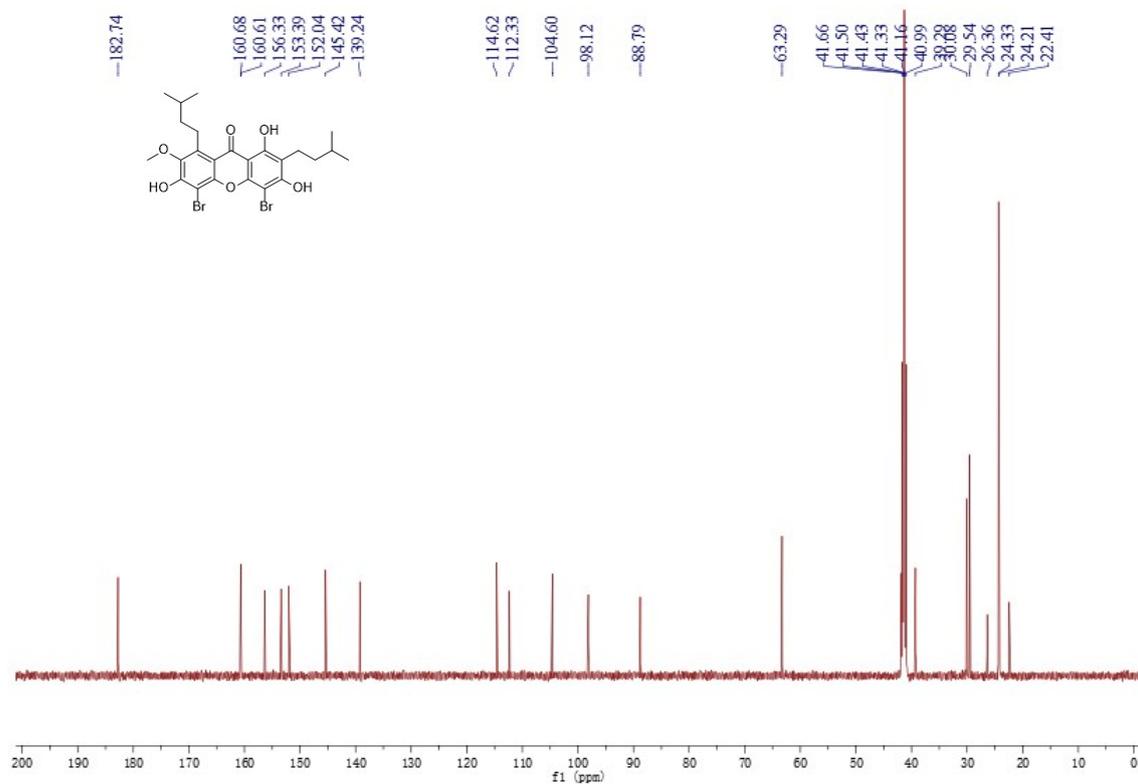


Figure 48S. Negative HR-ESIMS spectrum of compound 3d

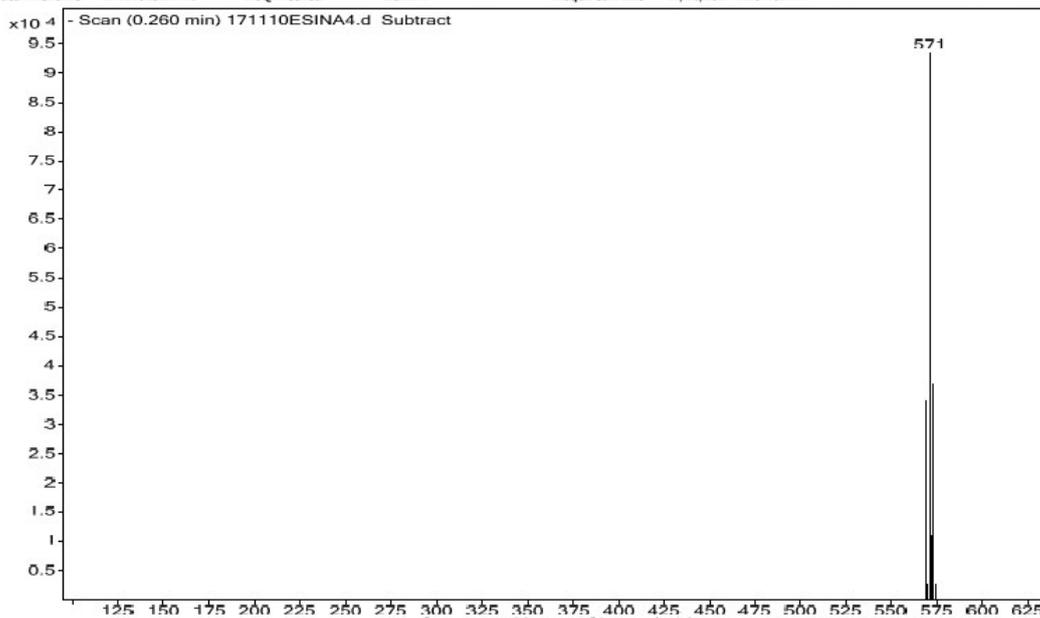


**Figure 49S.**  $^1\text{H}$  NMR spectrum ( $\text{DMSO-}d_6$ , 500 MHz) of compound **3e**



**Figure 50S.**  $^{13}\text{C}$  NMR spectrum ( $\text{DMSO-}d_6$ , 125 MHz) of compound **3e**

Sample Name ZQ-369 Instrument Name Agilent G6230 TOF MS User Name KIB IRM Calibration Status Success  
Data Filename 171110ESINA4.d ACQ Method ESIN.m Acquired Time 11/10/2017 11:37:02 AM



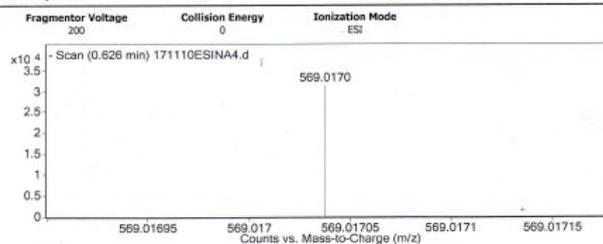
**Figure 51S.** Negative ESI-MS spectrum of compound **3e**

## Qualitative Analysis Report

Data Filename	171110ESINA4.d	Sample Name	ZQ-369
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESIN.m	Acquired Time	11/10/2017 11:37:02 AM
IRM Calibration Status	Success	DA Method	ESI.m

Sample Group: Info.  
 Acquisition SW: 6200 series TOF/6500 series  
 Version: Q-TOF B.05.01 (B5125.2)

### User Spectra



m/z	z	Abund	Formula	Ion
112.9856		1100.16		
268.9542		2169.93		
569.017	1	31477.38	C24 H27 Br2 O6	M-
570.0199	1	2968.07	C24 H27 Br2 O6	M-
571.0155	1	82986.43		
572.0181	1	10970.78		
573.0136	1	33935.88		
574.0155	1	2833.97		
1033.9881	1	29246.97		
1034.989	1	1577.2		

#### Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	2	10
Br	2	2

#### Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C24 H27 Br2 O6	569.0174	569.0170	0.4	0.8	10.5

**Figure 52S.** Negative HR-ESIMS spectrum of compound **3e**